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STIC Database Tracking Number: 203954

TO: Shailendra Kumar
Location: rem/5C03/5C18
Art Unit: 1621
Tuesday, October 10, 2006
Case Serial Number: 10/538328

From: Saloni Sharma
Location: Biotech-Chem Library
REM-1A64
Phone: (571)272-8601

saloni.sharma@uspto.gov

Search Notes

Examiner Kumar,

See attached results.

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Thank you for using STIC search services!

Saloni Sharma
Technical Information Specialist
STIC Biotech/Chem Library
(571)272-8601

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     (FILE 'HOME' ENTERED AT 13:36:45 ON 06 OCT 2006)

     FILE 'REGISTRY' ENTERED AT 13:36:50 ON 06 OCT 2006
L1              STRUCTURE UPLOADED
L2           50 SEA SSS SAM L1

     FILE 'STNGUIDE' ENTERED AT 13:37:18 ON 06 OCT 2006

     FILE 'REGISTRY' ENTERED AT 13:44:56 ON 06 OCT 2006
L3              STRUCTURE UPLOADED
L4           50 SEA SSS SAM L3

     FILE 'REGISTRY' ENTERED AT 13:56:52 ON 06 OCT 2006
L5              STRUCTURE UPLOADED
L6           50 SEA SSS SAM L5
                D QUE L3
L7           50 SEA SSS SAM L3
L8         5507 SEA SSS FUL L3
                SAVE L8 KUMAR328/A TEMP

     FILE 'HCAPLUS' ENTERED AT 13:58:02 ON 06 OCT 2006
L9          1777 SEA ABB=ON  PLU=ON  L8
L10          424 SEA ABB=ON  PLU=ON  L8 (L) (THU OR PKT OR DMA OR PAC OR
                BAC)/RL

     FILE 'REGISTRY' ENTERED AT 13:58:27 ON 06 OCT 2006

     FILE 'STNGUIDE' ENTERED AT 13:58:29 ON 06 OCT 2006

     FILE 'REGISTRY' ENTERED AT 14:02:07 ON 06 OCT 2006
L11             STRUCTURE UPLOADED
                D QUE L11
L12          50 SEA SUB=L8 SSS SAM L11
                D QUE L11
L13          50 SEA SUB=L8 SSS SAM L11
L14        5281 SEA SUB=L8 SSS FUL L11
                SAVE L14 SUBKEMAR/A TEMP

     FILE 'HCAPLUS' ENTERED AT 14:03:46 ON 06 OCT 2006
L15         1761 SEA ABB=ON  PLU=ON  L14

     FILE 'REGISTRY' ENTERED AT 14:03:53 ON 06 OCT 2006

     FILE 'HCAPLUS' ENTERED AT 14:04:29 ON 06 OCT 2006
                E US2005-538328/APPS
L16            1 SEA ABB=ON  PLU=ON  US2005-538328/AP
                D SCAN
                SEL RN L16

     FILE 'REGISTRY' ENTERED AT 14:04:57 ON 06 OCT 2006
                D E1-E60
L17           60 SEA ABB=ON  PLU=ON  (103904-73-0/BI OR 103904-74-1/BI OR
                117367-11-0/BI OR 134-11-2/BI OR 16611-84-0/BI OR 2100-31-4/BI
                OR 21615-34-9/BI OR 22910-60-7/BI OR 316128-15-1/BI OR
                320-51-4/BI OR 35151-93-0/BI OR 37330-39-5/BI OR 38449-25-1/BI
                OR 393-11-3/BI OR 42926-52-3/BI OR 451491-47-7/BI OR 485386-80-
                9/BI OR 485386-82-1/BI OR 54090-36-7/BI OR 57486-25-6/BI OR
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                579-75-9/BI OR 586976-24-1/BI OR 606-45-1/BI OR 6270-67-3/BI
                OR 6290-24-0/BI OR 63635-26-7/BI OR 654-70-6/BI OR 65446-29-9/B
                I OR 66849-11-4/BI OR 69-72-7/BI OR 709676-38-0/BI OR 709676-39
                -1/BI OR 709676-40-4/BI OR 709676-41-5/BI OR 709676-42-6/BI OR
                709676-43-7/BI OR 709676-44-8/BI OR 709676-45-9/BI OR 709676-46
                -0/BI OR 709676-47-1/BI OR 709676-48-2/BI OR 709676-49-3/BI OR
                709676-50-6/BI OR 709676-51-7/BI OR 709676-52-8/BI OR 709676-53
                -9/BI OR 709676-54-0/BI OR 709676-55-1/BI OR 709676-56-2/BI OR
                709676-57-3/BI OR 709676-58-4/BI OR 709676-59-5/BI OR 709676-60
                -8/BI OR 709676-61-9/BI OR 709676-62-0/BI OR 709676-63-1/BI OR
                710734-45-5/BI OR 79688-37-2/BI OR 86011-61-2/BI OR 9054-51-7/B
                I)
L18           22 SEA ABB=ON  PLU=ON  L17 AND L14
L19           22 SEA ABB=ON  PLU=ON  L17 AND L8
L20           38 SEA ABB=ON  PLU=ON  L17 NOT (L18 OR L19)
                D SCAN

     FILE 'HCAPLUS' ENTERED AT 14:06:17 ON 06 OCT 2006
L21            3 SEA ABB=ON  PLU=ON  L19
L22              ANALYZE PLU=ON  L15 1- RN :   51304 TERMS  (TERM LIMIT
                 EXCEEDED)
                 D

     FILE 'REGISTRY' ENTERED AT 14:07:53 ON 06 OCT 2006
L23            1 SEA ABB=ON  PLU=ON  87-17-2
                 D SCAN
L24            1 SEA ABB=ON  PLU=ON  69-72-7
                 D SCAN
L25            1 SEA ABB=ON  PLU=ON  62-53-3
                 D SCAN
L26            1 SEA ABB=ON  PLU=ON  110-91-8
                 D SCAN
L27            1 SEA ABB=ON  PLU=ON  110-89-4
                 D SCAN
L28            1 SEA ABB=ON  PLU=ON  98-88-4
                 D SCAN
L29            1 SEA ABB=ON  PLU=ON  65-45-2
                 D SCAN
L30            1 SEA ABB=ON  PLU=ON  108-95-2
                 D SCAN
L31            1 SEA ABB=ON  PLU=ON  50-78-2
                 D SCAN
L32            1 SEA ABB=ON  PLU=ON  98-80-6
                 D SCAN
L33            1 SEA ABB=ON  PLU=ON  L14 AND L23
L34         5280 SEA ABB=ON  PLU=ON  L14 NOT L23

     FILE 'HCAPLUS' ENTERED AT 14:11:17 ON 06 OCT 2006
L35         1116 SEA ABB=ON  PLU=ON  L34
L36          645 SEA ABB=ON  PLU=ON  L15 NOT L35
L37          820 SEA ABB=ON  PLU=ON  L23
L38           16 SEA ABB=ON  PLU=ON  L9 NOT L15
L39              ANALYZE PLU=ON  L38 1- RN :     342 TERMS
                 D

     FILE 'REGISTRY' ENTERED AT 14:12:22 ON 06 OCT 2006
L40            1 SEA ABB=ON  PLU=ON  2627-77-2
                 D SCAN
L41            1 SEA ABB=ON  PLU=ON  87-10-5
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                D SCAN
L42             1 SEA ABB=ON  PLU=ON  (L36 OR L37)

     FILE 'HCAPLUS' ENTERED AT 14:13:54 ON 06 OCT 2006
L43           820 SEA ABB=ON  PLU=ON  (L36 OR L37)
L44           821 SEA ABB=ON  PLU=ON  (L43 OR L16)
L45            17 SEA ABB=ON  PLU=ON  (L38 OR L16)
L46          1116 SEA ABB=ON  PLU=ON  (L35 OR L16)
L47               ANALYZE PLU=ON  L35 1- RN :   50407 TERMS  (TERM LIMIT
                  EXCEEDED)
                  D

     FILE 'REGISTRY' ENTERED AT 14:16:57 ON 06 OCT 2006
L48             1 SEA ABB=ON  PLU=ON  5538-51-2
                  D SCAN
L49             1 SEA ABB=ON  PLU=ON  100-39-0
                  D SCAN
L50             1 SEA ABB=ON  PLU=ON  26095-59-0
                  D SCAN
L51             2 SEA ABB=ON  PLU=ON  (L50 OR L23)
L52             1 SEA ABB=ON  PLU=ON  L34 AND L51
L53          5279 SEA ABB=ON  PLU=ON  L34 NOT L51
                  D SCAN L52

     FILE 'HCAPLUS' ENTERED AT 14:18:50 ON 06 OCT 2006
L54          1061 SEA ABB=ON  PLU=ON  L53
L55            55 SEA ABB=ON  PLU=ON  L35 NOT L54
L56           881 SEA ABB=ON  PLU=ON  L51
L57            61 SEA ABB=ON  PLU=ON  L52
L58            61 SEA ABB=ON  PLU=ON  (L55 OR L57)
L59            77 SEA ABB=ON  PLU=ON  (L58 OR L38)
L60           882 SEA ABB=ON  PLU=ON  (L56 OR L43 OR L44 OR L37 OR L36)
L61            63 SEA ABB=ON  PLU=ON  L59 AND (PY<2002 OR AY<2002 OR PRY<2002)
L62           790 SEA ABB=ON  PLU=ON  L60 AND (PY<2002 OR AY<2002 OR PRY<2002)
                  E HISTONE/CT
                  E E5+ALL
L63          1441 SEA ABB=ON  PLU=ON  "HISTONE ACETYLTRANSFERASE"+OLD,NT/CT
L64          1758 SEA ABB=ON  PLU=ON  (HISTONE ACETYLTRANSF?)/OBI,BI
L65             0 SEA ABB=ON  PLU=ON  L61 AND (L63 OR L64)
L66             0 SEA ABB=ON  PLU=ON  L62 AND (L63 OR L64)
L67             1 SEA ABB=ON  PLU=ON  L61 AND (AIDS? OR HIV? OR CANCER? OR
                  ASTHMA? OR GENE REGULATION?)/OBI,BI
L68            10 SEA ABB=ON  PLU=ON  L62 AND (AIDS? OR HIV? OR CANCER? OR
                  ASTHMA? OR GENE REGULATION?)/OBI,BI
L69            10 SEA ABB=ON  PLU=ON  (L68 OR L67)

     FILE 'REGISTRY' ENTERED AT 14:24:18 ON 06 OCT 2006

     FILE 'HCAPLUS' ENTERED AT 14:24:57 ON 06 OCT 2006
L70           423 SEA ABB=ON  PLU=ON  L14 (L) (THU OR DMA OR PKT OR PAC OR
                  BAC)/RL

     FILE 'STNGUIDE' ENTERED AT 14:25:13 ON 06 OCT 2006

     FILE 'HCAPLUS' ENTERED AT 14:25:31 ON 06 OCT 2006
L71            13 SEA ABB=ON  PLU=ON  (L21 OR L69)

     FILE 'STNGUIDE' ENTERED AT 14:25:44 ON 06 OCT 2006
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     FILE 'HCAPLUS' ENTERED AT 14:26:46 ON 06 OCT 2006
L72          126 SEA ABB=ON  PLU=ON  L51 (L) (THU OR DMA OR PKT OR PAC OR
                 BAC)/RL
L73           97 SEA ABB=ON  PLU=ON  L72 AND (PY<2002 OR AY<2002 OR PRY<2002)
L74          303 SEA ABB=ON  PLU=ON  L70 AND (PY<2002 OR AY<2002 OR PRY<2002)
L75          303 SEA ABB=ON  PLU=ON  L10 AND (PY<2002 OR AY<2002 OR PRY<2002)
L76          303 SEA ABB=ON  PLU=ON  (L73 OR L74 OR L75)
L77            0 SEA ABB=ON  PLU=ON  L76 AND (L63 OR L64)
                 E CANCER/CT
                 E E3+ALL
                 E E3+ALL
L*** DEL 430554 S E2+OLS,NT
                 E CANCER/CT
                 E E3+ALL
                 E E3+ALL
L78       432553 SEA ABB=ON  PLU=ON  NEOPLASM+OLD,NT/CT
                 E HIV/CT
                 E E3+ALL
                 E E3+ALL
L79        42075 SEA ABB=ON  PLU=ON  "HUMAN IMMUNODEFICIENCY VIRUS 1"+OLD,NT/CT

                 E HIV/CT
                 E E3+ALL
                 E E2+ALL
L80        52392 SEA ABB=ON  PLU=ON  "HUMAN IMMUNODEFICIENCY VIRUS"+OLD,NT/CT
                 E HIV/CT
                 E E4+ALL
                 E E2+ALL
L81        19610 SEA ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
                 E AIDS/CT
                 E E4+ALL
                 E E10+OLD,NT
L82        19610 SEA ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
                 E AIDS/CT
                 E E4+ALL
L83        19610 SEA ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
                 E AIDS/CT
                 E E5+ALL
L84          309 SEA ABB=ON  PLU=ON  "AIDS (DISEASE) (L) -RELATED COMPLEX"+OLD,N
                 T/CT
                 E AIDS/CT
                 E ASTHMA/CT
                 E E3+ALL
L85        21210 SEA ABB=ON  PLU=ON  ASTHMA+OLD,NT/CT
                 E ASTHMA/CT
                 E E4+ALL
L86         3251 SEA ABB=ON  PLU=ON  "ASTHMA (L) ALLERGIC"/CT
                 E ASTHMA/CT
                 E E5+ALL
L87          628 SEA ABB=ON  PLU=ON  "ASTHMA (L) OCCUPATIONAL"/CT
                 E ASTHMA/CT
L88     1001127 SEA ABB=ON  PLU=ON  (HIV? OR AIDS? OR ?ASTHMA? OR ?CANCER? OR
                 ?NEOPLASM? OR SARCOMA? OR LYMPHOMA? OR MELANOMA? OR TUMOR? OR
                 TUMOUR?)
L89     1001127 SEA ABB=ON  PLU=ON  (HIV? OR AIDS? OR ?ASTHMA? OR ?CANCER? OR
                 ?NEOPLASM? OR SARCOMA? OR LYMPHOMA? OR MELANOMA? OR TUMOR? OR
                 TUMOUR?)/OBI,BI
                 E TUMOR/CT
                 E E3+ALL
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                E E2+ALL
L90          34 SEA ABB=ON  PLU=ON  L76 AND (L77 OR L78 OR L79 OR L80 OR L81
                OR L82 OR L83 OR L84 OR L85 OR L86 OR L87 OR L88 OR L89)
L91          46 SEA ABB=ON  PLU=ON  (L90 OR L71)
L92          11 SEA ABB=ON  PLU=ON  L71 AND (PY<2002 OR AY<2002 OR PRY<2002)
L93          44 SEA ABB=ON  PLU=ON  (L90 OR L92)
L94          46 SEA ABB=ON  PLU=ON  (L91 OR L93)
L95          46 SEA ABB=ON  PLU=ON  (L16 OR L94)
L96          45 SEA ABB=ON  PLU=ON  L95 NOT L16
                E KUNDU T/AU
L97         107 SEA ABB=ON  PLU=ON  ("KUNDU T"/AU OR "KUNDU T K"/AU OR "KUNDU
                TAPAS K"/AU OR "KUNDU TAPAS KUMAR"/AU)
                E BALASUBRAMANYAM K/AU
L98          28 SEA ABB=ON  PLU=ON  ("BALASUBRAMANYAM K"/AU OR "BALASUBRAMANYAM
                 KARANAM"/AU OR "BALASUBRAMANYAM KARNAM"/AU)
                E SWAMINATHAN V/AU
L99         201 SEA ABB=ON  PLU=ON  ("SWAMINATHAN V"/AU OR "SWAMINATHAN V
                P"/AU OR "SWAMINATHAN V S"/AU OR "SWAMINATHAN V SRIRAMA"/AU OR
                "SWAMINATHAN VENKATESH"/AU)
L100         11 SEA ABB=ON  PLU=ON  (L97 AND (L98 OR L99)) OR (L98 AND L99)

     FILE 'HCAPLUS' ENTERED AT 14:36:48 ON 06 OCT 2006
                D QUE L100

=> file hcaplus
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FILE LAST UPDATED: 5 Oct 2006  (20061005/ED)

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=> d que l100
L97         107 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("KUNDU T"/AU OR "KUNDU T
                K"/AU OR "KUNDU TAPAS K"/AU OR "KUNDU TAPAS KUMAR"/AU)
L98          28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("BALASUBRAMANYAM K"/AU OR
                "BALASUBRAMANYAM KARANAM"/AU OR "BALASUBRAMANYAM KARNAM"/AU)
L99         201 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("SWAMINATHAN V"/AU OR
                "SWAMINATHAN V P"/AU OR "SWAMINATHAN V S"/AU OR "SWAMINATHAN V
                SRIRAMA"/AU OR "SWAMINATHAN VENKATESH"/AU)
L100         11 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L97 AND (L98 OR L99)) OR
                (L98 AND L99)
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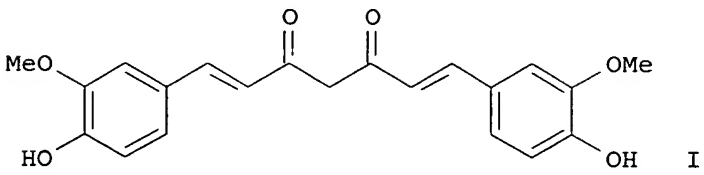
=> d ibib abs l100 tot

L100 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2006:79073 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 144:143100
TITLE: Use of curcumanoids as histone acetyltransferases inhibitors, and therapeutic uses
INVENTOR(S): ***Balasubramanyam, Karanam***; Varier, Radihika A.; M, Altaf; V, Swaminathan; ***Kundu, Tapas Kumar***
PATENT ASSIGNEE(S): India
SOURCE: U.S. Pat. Appl. Publ., 17 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006020027	A1	20060126	US 2005-149694	20050610
PRIORITY APPLN. INFO.:			IN 2004-CH544 A	20040611

OTHER SOURCE(S): MARPAT 144:143100
GI



I

AB The invention relates to the field of anticancer therapeutics, which can also be used to treat other diseases (e.g. HIV, cardiac hypertrophy, asthma) in humans. I and derivs. thereof are used to inhibit histone acetyltransferases.

L100 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:956223 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 143:300176
TITLE: Human histone chaperone nucleophosmin enhances acetylation-dependent chromatin transcription
AUTHOR(S): ***Swaminathan, V.***; Kishore, A. Hari; Febitha, K. K.; ***Kundu, Tapas K.***
CORPORATE SOURCE: Transcription and Disease Laboratory, Molecular Biology and Genetics Unit, Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, 64, India
SOURCE: Molecular and Cellular Biology (2005), 25(17), 7534-7545
CODEN: MCEBD4; ISSN: 0270-7306
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Histone chaperones are a group of proteins that aid in the dynamic chromatin organization during different cellular processes. Here, we report that the human histone chaperone nucleophosmin interacts with the core histones H3, H2B, and H4 but that this histone interaction is not sufficient to confer the chaperone activity. Significantly, nucleophosmin enhances the acetylation-dependent chromatin transcription and it becomes acetylated both in vitro and in vivo. Acetylation of nucleophosmin and the core histones was found to be essential for the enhancement of chromatin transcription. The acetylated NPM1 not only shows an increased affinity toward acetylated histones but also shows enhanced histone transfer ability. Presumably, nucleophosmin disrupts the nucleosomal structure in an acetylation-dependent manner, resulting in the transcriptional activation. These results establish nucleophosmin (NPM1) as a human histone chaperone that becomes acetylated, resulting in the enhancement of chromatin transcription.

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:451504 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 142:487548
TITLE: Polyisoprenylbenzophenones as inhibitors of histone acetyl transferases
INVENTOR(S): Tapas Kumar, Kundu; ***Balasubramanyam, Karanam***; Mantelingu, Kempegowda; Mohammad, Altaf; ***Swaminathan, Venkatesh***; Radhika, A. Varier
PATENT ASSIGNEE(S): Jawaharlal Nehru Centre for Advanced Scientific Research, India
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005047457	A2	20050526	WO 2004-IB52294	20041104
WO 2005047457	A3	20050804		
WO 2005047457	B1	20051201		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1694622	A2	20060830	EP 2004-799059	20041104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS				

PRIORITY APPLN. INFO.: IN 2003-CH929 A 20031113
WO 2004-IB52294 W 20041104
OTHER SOURCE(S): MARPAT 142:487548

AB The purification of prenylated benzophenones from the fruit rinds of Garcinia species and their evaluation as inhibitors of histone acetyltransferases

(HAT) p300 and PCAF. Prenylated benzophenones are potent HAT inhibitors of p300 (IC50 1 μM) and pCAF (IC50-15μM). The inhibitors significantly repress the p300 HAT dependent transcriptional activation from in vitro assembled chromatin template but have no effect on transcription from DNA. The compds. could be specific to HATs. Thus, these compds. should be useful as biol. switching mols. for evaluating the role of p300 and PCAF in cellular functions and may be useful as new chemical entities for the development of anticancer drugs.

L100 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2005:79644 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 142:233595
TITLE: The transcriptional coactivator p300 plays a critical role in the hypertrophic and protective pathways induced by phenylephrine in cardiac cells but is specific to the hypertrophic effect of urocortin
AUTHOR(S): Davidson, Sean M.; Townsend, Paul A.; Carroll, Chris; Yurek-George, Alexander; ***Balasubramanyam, Karanam; Kundu, Tapas K.***; Stephanou, Anastasis; Packham, Graham; Ganesan, A.; Latchman, David S.
CORPORATE SOURCE: Institute of Child Health, University College London, London, WC1N 1EH, UK
SOURCE: ChemBioChem (2005), 6(1), 162-170
CODEN: CBCHFX; ISSN: 1439-4227
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Anacardic acid is an alkylsalicylic acid obtained from cashewnut-shell liquid, and is a potent inhibitor of p300 histone acetyltransferase (HAT) activity. We have used anacardic acid to prevent the induction of hypertrophy in isolated neonatal rat cardiomyocytes. Hypertrophy was detected as an increase in cell size, the rearrangement of sarcomeres into a striated pattern, and the induction of embryonic genes β-MHC and ANF. The p300 inhibition was equally effective at preventing hypertrophy whether it was induced by treatment with the α1-adrenergic agonist, phenylephrine, or by treatment with urocortin, a member of the ACTH-releasing-factor family, which stimulates specific G protein-coupled receptors. Spiruchostatin A is a natural-product inhibitor of histone deacetylases (HDAC) similar to the depsipeptide FK 228 mol. We have recently synthesized spiruchostatin A and now show that, although HDACs act in opposition to HATs, spiruchostatin A has the same effect as anacardic acid, i.e., it prevents the induction of hypertrophy in response to phenylephrine or urocortin. Pretreatment with either phenylephrine or urocortin reduced the extent of death observed after the exposure of isolated cardiomyocytes to simulated ischemia and reoxygenation. Inhibition of p300 or HDAC activity eliminated the protection conferred by phenylephrine; however, it did not affect the protection conferred by urocortin. Therefore, it might eventually be possible to use chemical inhibitors such as these in a therapeutic setting to dissociate the protective effect and hypertrophic effect of urocortin, enhancing the survival of cardiomyocytes exposed to transient ischemia, while inhibiting the hypertrophic pathway that would otherwise be induced concurrently.
REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:1029058 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 142:149558

TITLE: Curcumin, a Novel p300/CREB-binding Protein-specific Inhibitor of Acetyltransferase, Represses the Acetylation of Histone/Nonhistone Proteins and Histone Acetyltransferase-dependent Chromatin Transcription
AUTHOR(S): ***Balasubramanyam, Karanam***; Varier, Radhika A.; Altaf, Mohammed; ***Swaminathan, Venkatesh***; Siddappa, Nagadenahalli B.; Ranga, Udaykumar; ***Kundu, Tapas K.***
CORPORATE SOURCE: Transcription and Disease Laboratory, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India
SOURCE: Journal of Biological Chemistry (2004), 279(49), 51163-51171
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Acetylation of histones and non-histone proteins is an important post-translational modification involved in the regulation of gene expression in eukaryotes and all viral DNA that integrates into the human genome (e.g. the human immunodeficiency virus). Dysfunction of histone acetyltransferases (HATs) is often associated with the manifestation of several diseases. In this respect, HATs are the new potential targets for the design of therapeutics. In this study,the authors report that curcumin (diferuloylmethane), a major curcumanoid in the spice turmeric, is a specific inhibitor of the p300/CREB-binding protein (CBP) HAT activity but not of p300/CBP-associated factor, in vitro and in vivo. Furthermore, curcumin could also inhibit the p300-mediated acetylation of p53 in vivo. It specifically represses the p300/CBP HAT activity-dependent transcriptional activation from chromatin but not a DNA template. It is significant that curcumin could inhibit the acetylation of HIV-Tat protein in vitro by p300 as well as proliferation of the virus, as revealed by the repression in syncytia formation upon curcumin treatment in SupT1 cells. Thus, non-toxic curcumin, which targets p300/CBP, may serve as a lead compound in combinatorial HIV therapeutics.
REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:677419 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 141:184475
TITLE: Implications of small molecule activators and inhibitors of histone acetyltransferases in chromatin therapy
AUTHOR(S): Varier, Radhika A.; ***Swaminathan, V.***; ***Balasubramanyam, Karanam***; ***Kundu, Tapas K.***
CORPORATE SOURCE: Transcription and Disease Laboratory, Molecular Biology and Genetics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India
SOURCE: Biochemical Pharmacology (2004), 68(6), 1215-1220
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review. Histone acetylation is a diagnostic feature of transcriptionally active chromatin. The group of enzymes, histone acetyltransferases (HATs), involved in this crucial step of gene

regulation, covalently modifies the N-terminal lysine residues of histones by the addition of an acetyl group from acetyl CoA. Dysfunction of these enzymes is often associated with several diseases, ranging from neurodegenerative disorders to cancer. These enzymes thus are potential new targets for therapeutics. We have discovered few small mol. compds., which target HATs and either activate or inhibit the enzyme potently. These compds. would be useful as biol. switching mols. for probing into the role of HATs in gene regulation and cell cycle and may be useful as new chemical entities for the development of new drugs.

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:617189 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 141:271145
TITLE: Polyisoprenylated Benzophenone, Garcinol, a Natural Histone Acetyltransferase Inhibitor, Represses Chromatin Transcription and Alters Global Gene Expression
AUTHOR(S): ***Balasubramanyam, Karanam***; Altaf, M.; Varier, Radhika A.; ***Swaminathan, V.***; Ravindran, Aarti; Sadhale, Parag P.; ***Kundu, Tapas K.***
CORPORATE SOURCE: Transcription and Disease Laboratory, Molecular Biology and Genetics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560064, India
SOURCE: Journal of Biological Chemistry (2004), 279(32), 33716-33726
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Histone acetylation is a diagnostic feature of transcriptionally active genes. The proper recruitment and function of histone acetyltransferases (HATs) and deacetylases (HDACs) are key regulatory steps for gene expression and cell cycle. Functional defects of either of these enzymes may lead to several diseases, including cancer. HATs and HDACs thus are potential therapeutic targets. Here we report that garcinol, a polyisoprenylated benzophenone derivative from Garcinia indica fruit rind, is a potent inhibitor of histone acetyltransferases p300 (IC50 ≈7 μM) and PCAF (IC50 ≈5 μM) both in vitro and in vivo. The kinetic anal. shows that it is a mixed type of inhibitor with an increased affinity for PCAF compared with p300. HAT activity-dependent chromatin transcription was strongly inhibited by garcinol, whereas transcription from DNA template was not affected. Furthermore, it was found to be a potent inducer of apoptosis, and it alters (predominantly down-regulates) the global gene expression in HeLa cells.

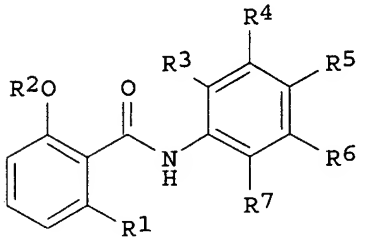
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2004:515708 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 141:67296
TITLE: Modulators (inhibitors/activators) of histone acetyltransferases
INVENTOR(S): ***Kundu, Tapas Kumar; Balasubramanyam, Karanam; Swaminathan, Venkatesh***
PATENT ASSIGNEE(S): Jawaharlal Nehru Centre for Advanced Scientific Research, India

SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004053140	A2	20040624	WO 2003-IN389	20031212
WO 2004053140	A3	20040916		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003288705	A1	20040630	AU 2003-288705	20031212
EP 1590318	A2	20051102	EP 2003-780608	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2006167107	A1	20060727	US 2005-538328	20051223
PRIORITY APPLN. INFO.:			IN 2002-MA925 A	20021212
			WO 2003-IN389 W	20031212

OTHER SOURCE(S): MARPAT 141:67296
GI



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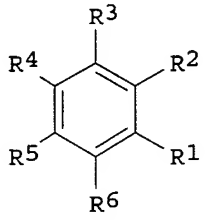


II

AB The invention provides the use of certain benzoic acid and benzamide compds. as modulators of enzymes histone acetyltransferases, which are involved in gene expression and cancer. Anacardic acid (6-pentadecylsalicylic acid), a major component of cashew nut shell liquid known to have antitumor activity, is shown to inhibit histone acetyltransferase activity of p300 and PCAF (p300/CBP-associated factor). Its amide derivs. shown an enhancement of p300 histone acetyltransferase activity with human core histones, and cannot affect the activity of PCAF even at high concns. Anacardic acid also inhibits p300 histone acetyltransferase-dependent transcription from the chromatin template but not DNA transcription, whereas the amide derivs. enhance chromatin transcription. Most analogs of the amide compds. show similar activity with regards to activation of histone acetylation, except of the CN-derivs., which predominantly enhances the acetylation of histone H3.

Thus, the present invention provides compds. of the general structures I (R1 = H, Me, Et Pr, iso-Pr, Bu, t-Bu, C8H18, C15C26, C15H28, C15H30, or C15H32; R2 = H, Me Et, Pr, iso-Pr, Bu, and t-butyl; R3 = R4 = R5 = R6 = R7 = H, Me, Et, Pr, iso-Pr, Bu, t-Bu, CF3, CCl3, CI3, F, Cl, I, NO2, CN) and II (R1 = R2 = R3 = R4 = R5 = R6 = H, CH3, hydroxyl, carboxylic, o-methoxy, o-ethoxy, n-propoxy, o-isopropoxy, n-butoxy, t-butoxy, C8H18, C15H26, C15H28, C15H30, or C15H32) in the treatment of diseases due to defects in gene regulation predominantly cancer.

L100 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:380722 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 139:207254
TITLE: Small Molecule Modulators of Histone Acetyltransferase p300
AUTHOR(S): ***Balasubramanyam, Karanam; Swaminathan, V.***; Ranganathan, Anupama; ***Kundu, Tapas K.***
CORPORATE SOURCE: ReNAXEIPRION SIA. Lv., Mol. Viol. Fwnwr. Unir., Jawaharlal Nehru Center for Advanced Scientific Research, Bangalore, 560064, India
SOURCE: Journal of Biological Chemistry (2003), 278(21), 19134-19140
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Histone acetyltransferases (HATs) are a group of enzymes that play a significant role in the regulation of gene expression. These enzymes covalently modify the N-terminal lysine residues of histones by the addition of acetyl groups from acetyl-CoA. Dysfunction of these enzymes is often associated with the manifestation of several diseases, predominantly cancer. Here we report that anacardic acid from cashew nut shell liquid is a potent inhibitor of p300 and p300/CBP-associated factor histone acetyltransferase activities. Although it does not affect DNA transcription, HAT-dependent transcription from a chromatin template was strongly inhibited by anacardic acid. Furthermore, we describe the design and synthesis of an amide derivative N-(4-chloro-3-trifluoromethyl-phenyl)-2-ethoxy-6-pentadecyl-benzamide (CTPB) using anacardic acid as a synthon, which remarkably activates p300 HAT activity but not that of p300/CBP-associated factor. Although CTPB does not affect DNA transcription, it enhances the p300 HAT-dependent transcriptional activation from in vitro assembled chromatin template. However, it has no effect on histone deacetylase activity. These compds. would be useful as biol. switching mols. for probing into the role of p300 in transcriptional studies and may also be useful as new chemical entities for the development of anticancer drugs.
REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:361004 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 137:121253
TITLE: Effect of phosphorylation on the structure and fold of transactivation domain of p53
AUTHOR(S): Kar, Sanchari; Sakaguchi, Kazuyasu; Shimohigashi, Yasuyuki; Samaddar, Soma; Banerjee, Raja; Basu, Gautam; ***Swaminathan, V.***; ***Kundu, Tapas K.***; Roy, Siddhartha
CORPORATE SOURCE: Department of Biophysics, Bose Institute, Calcutta, 700 054, India

SOURCE: Journal of Biological Chemistry (2002), 277(18), 15579-15585
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several phosphorylations are known to occur in the N-terminal transactivation domain of human p53. To explore the structural effects of these phosphorylations, the authors have chemical synthesized the unphosphorylated p53-(1-39) and its three phosphorylated analogs, phosphorylated at Ser 15, Thr 18, and Ser 20. P53-(1-39) and its Ser 15 and Thr 18 phosphorylated analogs were tested for interaction with p300. The order of binding affinities was similar to that derived from biochem. expts. with the whole protein, indicating functional integrity of the domain. Differences in chemical shifts and coupling consts. indicate significant structural changes upon phosphorylations. The single tryptophan in the unphosphorylated domain has an emission maximum and a Stern-Volmer constant that are characteristics of tryptophans situated in protein interiors. The diffusion constant is monomer-like, with an axial ratio of 1:7.5, indicating a significant degree of compaction. Upon phosphorylations, the emission maximum and diffusion constant change significantly toward values that indicate more open conformations. Binding of the hydrophobic probe bis-1-anilino-8-naphthalenesulfonate to the unphosphorylated and one of the phosphorylated domains is also significantly different, suggesting different conformations. The authors propose that phosphorylations switch the largely folded transactivation domain to more open conformations that interact with transcription factors such as p300/cAMP-responsive element-binding protein-binding protein, leading to enhancement of gene expression.

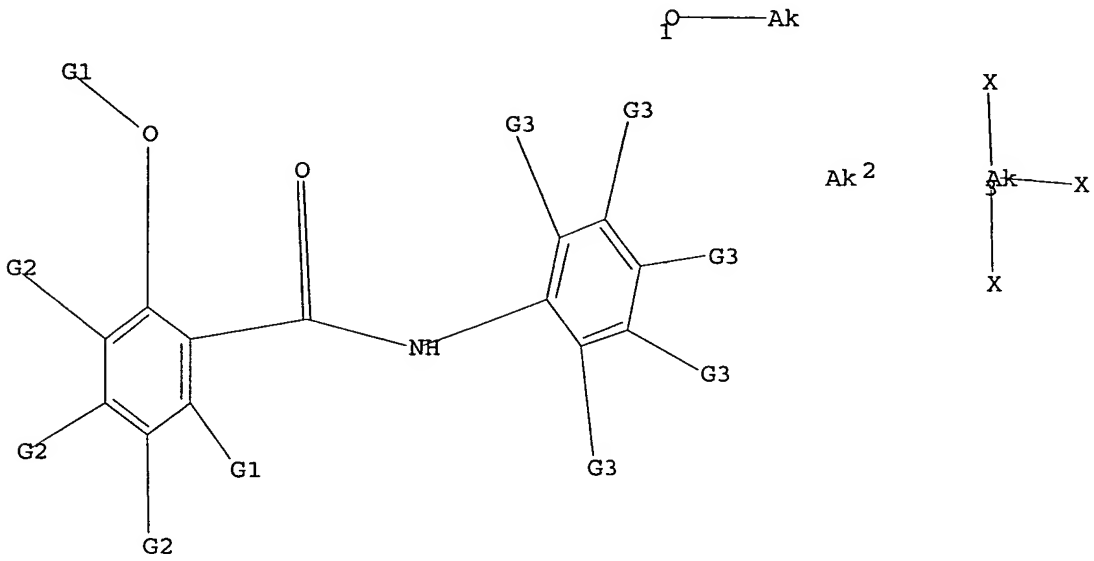
REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L100 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:395106 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:118457
TITLE: p300-mediated acetylation of human transcriptional coactivator PC4 is inhibited by phosphorylation
AUTHOR(S): Kumar, B. R. Prashanth; ***Swaminathan, V.***; Banerjee, Sourav; ***Kundu, Tapas K.***
CORPORATE SOURCE: Transcription and Disease Laboratory, Molecular Biology and Genetics Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, 560 064, India
SOURCE: Journal of Biological Chemistry (2001), 276(20), 16804-16809
CODEN: JBCHA3; ISSN: 0021-9258
PUBLISHER: American Society for Biochemistry and Molecular Biology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The human pos. coactivator 4 (PC4) acts as a general coactivator for activator-dependent transcription, the activity of which is regulated neg. by phosphorylation. We report here that PC4 can be acetylated specifically by another coactivator, p300. Interestingly, phosphorylation of PC4 by casein kinase II inhibits the p300-mediated acetylation. Mass spectral anal. revealed that there are at least two lysine residues acetylated in PC4, as a result of which its DNA binding activity is stimulated.

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d que l96
L3 STR



G1 Ak,H

G2 Ak,H, [@1]

G3 X,CN,NO2,H, [@2], [@3]

Structure attributes must be viewed using STN Express query preparation.

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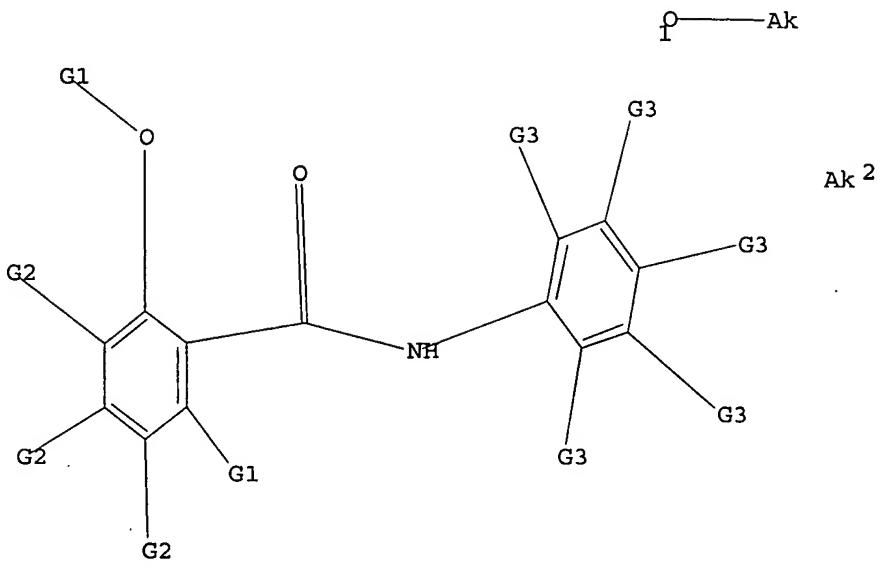
L9 1777 SEA FILE=HCAPLUS ABB=ON PLU=ON L8
L10 424 SEA FILE=HCAPLUS ABB=ON PLU=ON L8 (L) (THU OR PKT OR DMA OR PAC OR BAC)/RL
L11 STR



G1 Ak,H

G2 Ak,H, [@1]

G3 H,CF3,CCl3,CI3,CN,NO2,Cl,F,I, [@2]

Structure attributes must be viewed using STN Express query preparation.

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L15 1761 SEA FILE=HCAPLUS ABB=ON PLU=ON L14

L16 1 SEA FILE=HCAPLUS ABB=ON PLU=ON US2005-538328/AP

L17 60 SEA FILE=REGISTRY ABB=ON PLU=ON (103904-73-0/BI OR 103904-74-1/BI OR 117367-11-0/BI OR 134-11-2/BI OR 16611-84-0/BI OR 2100-31-4/BI OR 21615-34-9/BI OR 22910-60-7/BI OR 316128-15-1/BI OR 320-51-4/BI OR 35151-93-0/BI OR 37330-39-5/BI OR 38449-25-1/BI OR 393-11-3/BI OR 42926-52-3/BI OR 451491-47-7/BI OR 485386-80-9/BI OR 485386-82-1/BI OR 54090-36-7/BI OR 57486-25-6/BI OR 579-75-9/BI OR 586976-24-1/BI OR 606-45-1/BI OR 6270-67-3/BI OR 6290-24-0/BI OR 63635-26-7/BI OR 654-70-6/BI OR 65446-29-9/BI OR 66849-11-4/BI OR 69-72-7/BI OR 709676-38-0/BI OR 709676-39-1/BI OR 709676-40-4/BI OR 709676-41-5/BI OR 709676-42-6/BI OR 709676-43-7/BI OR 709676-44-8/BI OR 709676-45-9/BI OR 709676-46-0/BI OR 709676-47-1/BI OR 709676-48-2/BI OR 709676-49-3/BI OR 709676-50-6/BI OR 709676-51-7/BI OR 709676-52-8/BI OR 709676-53-9/BI OR 709676-54-0/BI OR 709676-55-1/BI OR 709676-56-2/BI OR 709676-57-3/BI OR 709676-58-4/BI OR 709676-59-5/BI OR 709676-60-8/BI OR 709676-61-9/BI OR 709676-62-0/BI OR 709676-63-1/BI OR 710734-45-5/BI OR 79688-37-2/BI OR 86011-61-2/BI OR 9054-51-7/BI)

L19 22 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND L8

L21 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L19

L23 1 SEA FILE=REGISTRY ABB=ON PLU=ON 87-17-2

L34 5280 SEA FILE=REGISTRY ABB=ON PLU=ON L14 NOT L23

L35 1116 SEA FILE=HCAPLUS ABB=ON PLU=ON L34

L36 645 SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L35

L37 820 SEA FILE=HCAPLUS ABB=ON PLU=ON L23

L38 16 SEA FILE=HCAPLUS ABB=ON PLU=ON L9 NOT L15

L43 820 SEA FILE=HCAPLUS ABB=ON PLU=ON (L36 OR L37)

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L50            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  26095-59-0
L51            2 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L50 OR L23)
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L53         5279 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 NOT L51
L54         1061 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L53
L55           55 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L35 NOT L54
L56          881 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L51
L57           61 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L52
L58           61 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L55 OR L57)
L59           77 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L58 OR L38)
L60          882 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L56 OR L43 OR L44 OR L37 OR
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L61           63 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L59 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
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L77            0 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L76 AND (L63 OR L64)
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L80        52392 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HUMAN IMMUNODEFICIENCY
                 VIRUS"+OLD,NT/CT
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L86         3251 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "ASTHMA (L) ALLERGIC"/CT
L87          628 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "ASTHMA (L) OCCUPATIONAL"/CT
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                 OR TUMOR? OR TUMOUR?)/OBI,BI
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                L89)
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                OR PRY<2002)
L93           44 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L90 OR L92)
L94           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L91 OR L93)
L95           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L16 OR L94)
L96           45 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L95 NOT L16


=> s l96 not l100
L101          44 L96 NOT L100

=> d que l101
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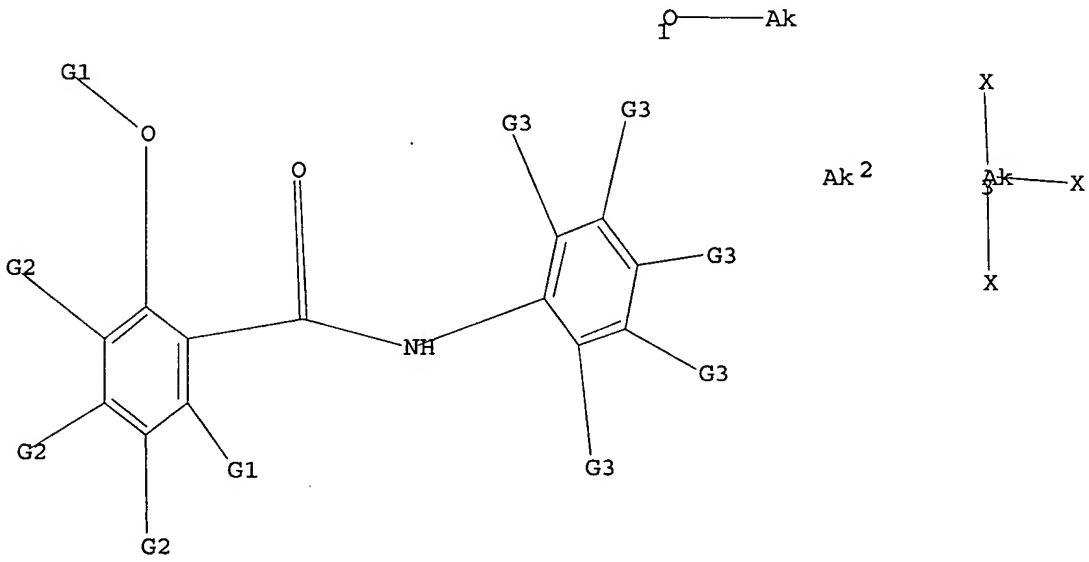


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G1 Ak,H
G2 Ak,H,[@1]
G3 X,CN,NO2,H,[@2],[@3]


Structure attributes must be viewed using STN Express query preparation.
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L9          1777 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8
L10          424 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 (L) (THU OR PKT OR DMA OR
                 PAC OR BAC)/RL
L11              STR
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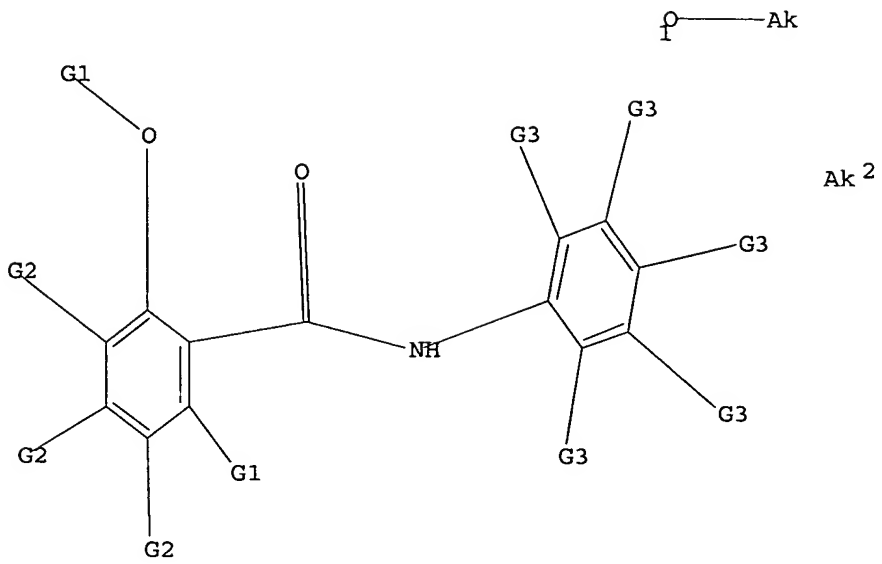

G1 Ak,H

G2 Ak,H, [@1]

G3 H,CF3,CCl3,CI3,CN,NO2,Cl,F,I, [@2]

Structure attributes must be viewed using STN Express query preparation.

L14	5281	SEA FILE=REGISTRY SUB=L8 SSS FUL L11
L15	1761	SEA FILE=HCAPLUS ABB=ON PLU=ON L14
L16	1	SEA FILE=HCAPLUS ABB=ON PLU=ON US2005-538328/AP
L17	60	SEA FILE=REGISTRY ABB=ON PLU=ON (103904-73-0/BI OR 103904-74-1/BI OR 117367-11-0/BI OR 134-11-2/BI OR 16611-84-0/BI OR 2100-31-4/BI OR 21615-34-9/BI OR 22910-60-7/BI OR 316128-15-1/BI OR 320-51-4/BI OR 35151-93-0/BI OR 37330-39-5/BI OR 38449-25-1/BI OR 393-11-3/BI OR 42926-52-3/BI OR 451491-47-7/BI OR 485386-80-9/BI OR 485386-82-1/BI OR 54090-36-7/BI OR 57486-25-6/BI OR 579-75-9/BI OR 586976-24-1/BI OR 606-45-1/BI OR 6270-67-3/BI OR 6290-24-0/BI OR 63635-26-7/BI OR 654-70-6/BI OR 65446-29-9/BI OR 66849-11-4/BI OR 69-72-7/BI OR 709676-38-0/BI OR 709676-39-1/BI OR 709676-40-4/BI OR 709676-41-5/BI OR 709676-42-6/BI OR 709676-43-7/BI OR 709676-44-8/BI OR 709676-45-9/BI OR 709676-46-0/BI OR 709676-47-1/BI OR 709676-48-2/BI OR 709676-49-3/BI OR 709676-50-6/BI OR 709676-51-7/BI OR 709676-52-8/BI OR 709676-53-9/BI OR 709676-54-0/BI OR 709676-55-1/BI OR 709676-56-2/BI OR 709676-57-3/BI OR 709676-58-4/BI OR 709676-59-5/BI OR 709676-60-8/BI OR 709676-61-9/BI OR 709676-62-0/BI OR 709676-63-1/BI OR 710734-45-5/BI OR 79688-37-2/BI OR 86011-61-2/BI OR 9054-51-7/BI)
L19	22	SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND L8
L21	3	SEA FILE=HCAPLUS ABB=ON PLU=ON L19
L23	1	SEA FILE=REGISTRY ABB=ON PLU=ON 87-17-2
L34	5280	SEA FILE=REGISTRY ABB=ON PLU=ON L14 NOT L23
L35	1116	SEA FILE=HCAPLUS ABB=ON PLU=ON L34
L36	645	SEA FILE=HCAPLUS ABB=ON PLU=ON L15 NOT L35
L37	820	SEA FILE=HCAPLUS ABB=ON PLU=ON L23
L38	16	SEA FILE=HCAPLUS ABB=ON PLU=ON L9 NOT L15
L43	820	SEA FILE=HCAPLUS ABB=ON PLU=ON (L36 OR L37)

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L50            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  26095-59-0
L51            2 SEA FILE=REGISTRY ABB=ON  PLU=ON  (L50 OR L23)
L52            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 AND L51
L53         5279 SEA FILE=REGISTRY ABB=ON  PLU=ON  L34 NOT L51
L54         1061 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L53
L55           55 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L35 NOT L54
L56          881 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L51
L57           61 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L52
L58           61 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L55 OR L57)
L59           77 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L58 OR L38)
L60          882 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L56 OR L43 OR L44 OR L37 OR
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L61           63 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L59 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
L62          790 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L60 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
L63         1441 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HISTONE ACETYLTRANSFERASE"+OL
                 D,NT/CT
L64         1758 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (HISTONE ACETYLTRANSF?)/OBI,BI

L67            1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L61 AND (AIDS? OR HIV? OR
                 CANCER? OR ASTHMA? OR GENE REGULATION?)/OBI,BI
L68           10 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L62 AND (AIDS? OR HIV? OR
                 CANCER? OR ASTHMA? OR GENE REGULATION?)/OBI,BI
L69           10 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L68 OR L67)
L70          423 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14 (L) (THU OR DMA OR PKT OR
                 PAC OR BAC)/RL
L71           13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L21 OR L69)
L72          126 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L51 (L) (THU OR DMA OR PKT OR
                 PAC OR BAC)/RL
L73           97 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L72 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
L74          303 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L70 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
L75          303 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L10 AND (PY<2002 OR AY<2002
                 OR PRY<2002)
L76          303 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L73 OR L74 OR L75)
L77            0 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L76 AND (L63 OR L64)
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L79        42075 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HUMAN IMMUNODEFICIENCY VIRUS
                 1"+OLD,NT/CT
L80        52392 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "HUMAN IMMUNODEFICIENCY
                 VIRUS"+OLD,NT/CT
L81        19610 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
L82        19610 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
L83        19610 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "AIDS (DISEASE)"+OLD,NT/CT
L84          309 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "AIDS (DISEASE) (L) -RELATED
                 COMPLEX"+OLD,NT/CT
L85        21210 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ASTHMA+OLD,NT/CT
L86         3251 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "ASTHMA (L) ALLERGIC"/CT
L87          628 SEA FILE=HCAPLUS ABB=ON  PLU=ON  "ASTHMA (L) OCCUPATIONAL"/CT
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                 ?CANCER? OR ?NEOPLASM? OR SARCOMA? OR LYMPHOMA? OR MELANOMA?
                 OR TUMOR? OR TUMOUR?)
L89      1001127 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (HIV? OR AIDS? OR ?ASTHMA? OR
                 ?CANCER? OR ?NEOPLASM? OR SARCOMA? OR LYMPHOMA? OR MELANOMA?
                 OR TUMOR? OR TUMOUR?)/OBI,BI
L90           34 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L76 AND (L77 OR L78 OR L79 OR
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                L80 OR L81 OR L82 OR L83 OR L84 OR L85 OR L86 OR L87 OR L88 OR
                L89)
L91          46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L90 OR L71)
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L93          44 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L90 OR L92)
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L95          46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L16 OR L94)
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L97         107 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("KUNDU T"/AU OR "KUNDU T
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L98          28 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("BALASUBRAMANYAM K"/AU OR
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L99         201 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ("SWAMINATHAN V"/AU OR
                "SWAMINATHAN V P"/AU OR "SWAMINATHAN V S"/AU OR "SWAMINATHAN V
                SRIRAMA"/AU OR "SWAMINATHAN VENKATESH"/AU)
L100         11 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L97 AND (L98 OR L99)) OR
                (L98 AND L99)
L101         44 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L96 NOT L100


=> d ibib abs hitind hitstr l101 tot

L101 ANSWER 1 OF 44  HCAPLUS  COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER:         2003:485719  HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER:          139:53315
TITLE:                    Preparation of N-sulfonylated dipeptide derivatives as
                          inhibitors of leukocyte adhesion mediated by VLA-4
INVENTOR(S):              Thorsett, Eugene D.; Semko, Christopher M.; Pleiss,
                          Michael A.; Kreft, Anthony; Konradi, Andrei W.; Grant,
                          Francine S.; Baudy, Reinhardt Bernhard; Sarantakis,
                          Dimitrios
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 127,346,
                          abandoned.
                          CODEN: USXXAM
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.         DATE
     ---------------      ----   --------    --------------------    --------
     US 6583139            B1    20030624    US 2000-688820          20001017 <--
     US 2004006093         A1    20040108    US 2003-382988          20030307 <--
PRIORITY APPLN. INFO.:                       US 1997-104592P      P  19970731 <--
                                             US 1998-127346       B1 19980731 <--
                                             US 2000-688820       A1 20001017 <--
OTHER SOURCE(S):          MARPAT 139:53315
AB   Disclosed are N-sulfonylated dipeptides R1SO2NR2CHR3-Q-CHR5CO2H [R1, R3 =
     (un)substituted alkyl, aryl, cycloalkyl, heterocyclyl or heteroaryl; R2 =
     H, (un)substituted cycloalkenyl, or any group given for R1; or R2 may form
     an (un)substituted heterocyclic ring with R1 or R3; R5 = CH2-X', where X'
     = H, OH, acylamino, (cyclo)alkyl, alkoxy, aryloxy, (hetero)aryl,
     aryloxyalkyl, carboxy, carboxyalkyl, etc.; Q = C(X)NR7; R7 = H, alkyl; X =
     O, S (with provisos)] which bind VLA-4.  Certain of these compds. also
     inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated
     by VLA-4.  Such compds. are useful in the treatment of inflammatory
     diseases in a mammalian patient, e.g., human, such as asthma,
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Alzheimer's disease, atherosclerosis, ***AIDS*** dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, ***tumor*** metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis. Thus, coupling of N-tosyl-L-proline with L-tyrosine Me ester, followed by reaction with (1-bromoethyl)benzene and saponification, afforded N-tosyl-L-prolyl-4-(α-methylbenzyloxy)-L-phenylalanine.

IC ICM A61K031-54
ICS C07D217-02; C07D277-02; C07D279-12; C07D295-00

INCL 514227500; 514307000; 514365000; 544059000; 544316000; 546147000; 548146000; 560016000

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 63

IT ***Neoplasm***
(metastasis; preparation of N-sulfonylated dipeptide derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

IT ***AIDS (disease)***
Alzheimer's disease
Anti-***AIDS*** agents
Anti-Alzheimer's agents
Anti-ischemic agents
Antiarteriosclerotics
Antiasthmatics
Antidiabetic agents
Antirheumatic agents
Antitumor agents
Asthma
Atherosclerosis
Dermatitis
Diabetes mellitus
Encephalitis
Human
Meningitis
Multiple sclerosis
Psoriasis
Rheumatoid arthritis
Transplant and Transplantation
(preparation of N-sulfonylated dipeptide derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

IT 4902-49-2P 220202-29-9P 220302-20-5P 220302-23-8P 220302-24-9P
220302-25-0P 220302-26-1P 220302-27-2P 220302-28-3P 220302-29-4P
220302-30-7P 220302-31-8P 220302-32-9P 220302-33-0P 220302-34-1P
220302-35-2P 220302-36-3P 220302-37-4P 220302-38-5P 220302-39-6P
220302-40-9P 220302-41-0P 220302-42-1P 220302-43-2P 220302-44-3P
220302-45-4P 220302-46-5P 220302-47-6P 220302-48-7P 220302-49-8P
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220302-55-6P 220302-56-7P 220302-57-8P 220302-58-9P 220302-59-0P
220302-61-4P 220302-63-6P 220302-64-7P 220302-65-8P 220302-67-0P
220302-68-1P 220302-69-2P 220302-70-5P 220302-71-6P 220302-72-7P
220302-73-8P 220302-74-9P 220302-75-0P 220302-76-1P 220302-77-2P
220302-78-3P 220302-79-4P 220302-80-7P 220302-81-8P 220302-82-9P
220302-83-0P 220302-84-1P 220302-85-2P 220302-86-3P 220302-87-4P
220302-88-5P 220302-89-6P 220302-90-9P ***220302-91-0P***
220302-92-1P 220302-93-2P 220302-94-3P ***220302-95-4P***
220302-96-5P 220302-97-6P 220302-98-7P 220303-00-4P 220303-01-5P
220303-02-6P 220303-03-7P 220303-04-8P 220303-05-9P 220303-06-0P
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220303-12-8P 220303-13-9P 220303-14-0P 220303-15-1P 220303-16-2P
220303-17-3P 220303-18-4P 220303-19-5P 220303-20-8P 220303-21-9P

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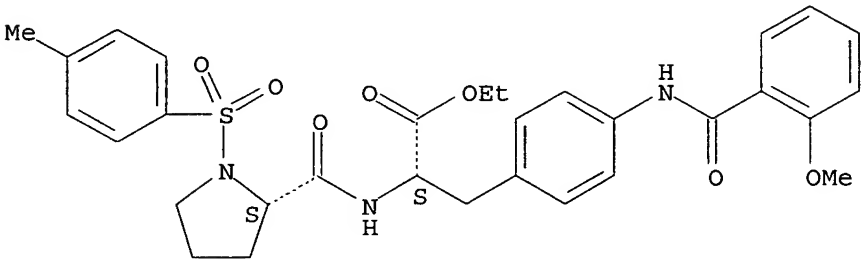
220303-54-8P 220303-55-9P 220303-56-0P 220303-57-1P 220303-58-2P
220303-59-3P 220303-60-6P 220303-61-7P 220303-62-8P 220303-63-9P
220337-23-5P 548464-65-9P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-sulfonylated dipeptide derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

IT ***220302-91-0P 220302-95-4P***
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-sulfonylated dipeptide derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

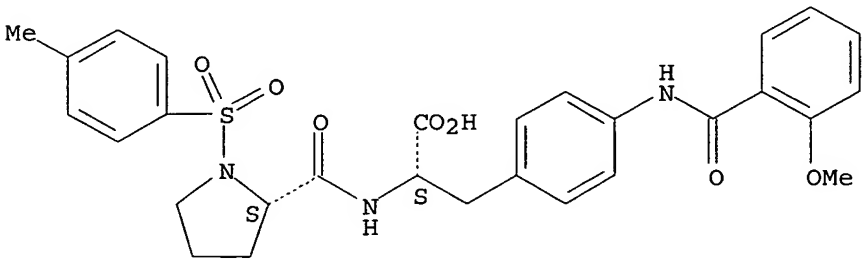
RN 220302-91-0 HCAPLUS
CN L-Phenylalanine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-4-[(2-methoxybenzoyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 220302-95-4 HCAPLUS
CN L-Phenylalanine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-4-[(2-methoxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 87 THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 2 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:454113 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 139:36517
TITLE: Preparation of 1-phenyl-oxazolidine-2-ones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases
INVENTOR(S): Buchstaller, Hans-Peter; Poeschke, Oliver; Willems, Andreas
PATENT ASSIGNEE(S): Merck Patent Gmbh, Germany
SOURCE: PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2003047572	A1	20030612	WO 2002-EP12162		20021031	<--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW						
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG						
DE 10159453	A1	20030618	DE 2001-10159453		20011204	<--
AU 2002346812	A1	20030617	AU 2002-346812		20021031	<--
PRIORITY APPLN. INFO.:			DE 2001-10159453	A	20011204	<--
			WO 2002-EP12162	W	20021031	

OTHER SOURCE(S): MARPAT 139:36517
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = alkyl, (un)substituted cycloalkyl, Ph, etc.; R2 = H2NC(=NH)] and their pharmaceutically acceptable salts were prepared For example, coupling of benzoic acid II, prepared from 3-hydroxybenzoic acid 2-propenyl ester in 3-steps, and phenylamine, followed by Raney-Ni reduction afforded phenyloxazolidinone III acetate. Compds. I are claimed useful as protease M inhibitors (no data provided).
IC ICM A61K031-42
ICS A61K031-422; C07D263-24; C07D413-12
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT Nervous system, disease
(degeneration; preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)
IT Alzheimer's disease
Anti-Alzheimer's agents
Antiparkinsonian agents
Antitumor agents

Cognition enhancers
Human
Mammary gland, neoplasm
Neoplasm
Ovary, neoplasm
Pancreas, neoplasm
Parkinson's disease
(preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT Integrins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT 540505-46-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide 540505-48-4P, N-Butyl-3-[3-(4-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide 540505-50-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-diethylbenzamide 540505-52-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dipropylbenzamide 540505-54-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dibutylbenzamide 540505-56-4P 540505-58-6P 540505-60-0P 540505-62-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-cyclohexylbenzamide 540505-64-4P, N-Benzyl-3-[3-(4-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide 540505-66-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-ethylbenzamide 540505-68-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-propylbenzamide 540505-70-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-fluorobenzyl)benzamide 540505-72-4P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-fluorobenzyl)benzamide 540505-74-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methylbenzyl)benzamide 540505-76-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxybenzyl)benzamide 540505-78-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxybenzyl)benzamide 540505-80-4P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-trifluoromethoxybenzyl)benzamide 540505-82-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenethylbenzamide 540505-84-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxyphenethyl)benzamide 540505-86-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3,4-dimethoxyphenethyl)benzamide 540505-88-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenethyl)benzamide 540505-90-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-fluorophenyl)benzamide 540505-92-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methylphenyl)benzamide 540505-94-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxyphenyl)benzamide 540505-96-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide 540506-00-1P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3,4,5-trimethoxyphenyl)benzamide 540506-02-3P 540506-04-5P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenyl)benzamide 540506-06-7P 540506-08-9P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide 540506-10-3P 540506-12-5P, 5-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-2-methyl-1-propyl-1H-indol-3-carboxylic acid ethyl ester 540506-14-7P 540506-16-9P 540506-18-1P 540506-20-5P 540506-22-7P 540506-24-9P 540506-26-1P 540506-28-3P, [4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetic acid ethyl ester 540506-30-7P, N-[4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-

ylmethoxy]phenyl]acetamide ***540506-32-9P***, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide 540506-34-1P 540506-36-3P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-4-methoxybenzoic acid methyl ester 540506-38-5P 540506-40-9P 540506-42-1P 540506-44-3P 540506-46-5P, 4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid ethyl ester 540506-48-7P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid methyl ester 540506-50-1P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid ethyl ester 540506-53-4P 540506-55-6P 540506-57-8P 540506-59-0P 540506-61-4P, 4-[5-(Chroman-6-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-63-6P 540506-65-8P, 3-[4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]propionic acid methyl ester 540506-67-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid methyl ester 540506-69-2P 540506-71-6P 540506-73-8P, 4-[5-(1H-Indol-5-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-75-0P, 4-[2-Oxo-5-(4-phenoxyphenoxymethyl)oxazolidin-3-yl]benzamidin 540506-77-2P 540506-79-4P, 4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-propylbenzoic acid methyl ester 540506-81-8P, 4-[2-Oxo-5-(4-propionylphenoxymethyl)oxazolidin-3-yl]benzamidin 540506-83-0P, 4-[5-(4-Acetyl-2-methoxyphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-85-2P, 4-[5-(4-Propionyl-2-methoxyphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-87-4P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-bis(3-methylbutyl)benzamide 540506-89-6P, N-[4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-methylnaphthalen-1-yl]acetamide 540506-91-0P, 4-[2-Oxo-5-(2-trifluoromethylphenoxymethyl)oxazolidin-3-yl]benzamidin 540506-93-2P, 4-[5-(Biphenyl-3-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-95-4P, 4-[2-Oxo-5-(3-phenoxyphenoxymethyl)oxazolidin-3-yl]benzamidin 540506-97-6P, 4-[5-(Biphenyl-4-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540506-99-8P, N-[2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide 540507-01-5P, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-4-methoxybenzoic acid methyl ester 540507-03-7P, 3-[2-Oxo-5-(4-propoxyphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-05-9P, 3-[2-Oxo-5-[4-(4-propylcyclohexyl)phenoxymethyl]oxazolidin-3-yl]benzamidin 540507-07-1P, 3-[5-(Naphthalen-1-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-11-7P, 3-[5-(Naphthalen-2-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-13-9P, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid ethyl ester 540507-15-1P, 3-[5-(4-Cyclohexylphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-17-3P 540507-19-5P, 3-[5-(2-Benzyl-4-chlorophenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-22-0P 540507-25-3P, 4-[5-(2-Acetylphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-27-5P, 4-[5-(4-tert-Butylphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-29-7P ***540507-31-1P***, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide 540507-33-3P 540507-36-6P, 3-[4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]propionic acid methyl ester 540507-38-8P 540507-40-2P 540507-42-4P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid methyl ester 540507-46-8P 540507-48-0P, N-[4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide 540507-50-4P, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid methyl ester 540507-52-6P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzoic acid ethyl ester 540507-55-9P, 3-[2-Oxo-5-(3-trifluoromethylphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-57-1P, 3-[2-Oxo-5-(4-phenoxyphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-59-3P,

N-[2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide 540507-62-8P 540507-64-0P, 3-[2-Oxo-5-(quinolin-6-yloxymethyl)oxazolidin-3-yl]benzamidin 540507-66-2P 540507-70-8P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-propylbenzoic acid methyl ester 540507-72-0P, 3-[2-Oxo-5-(4-propionylphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-74-2P, 3-[5-(4-Acetyl-2-methoxyphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-76-4P, 3-[2-Oxo-5-(3-phenoxyphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-77-5P, 3-[5-(Biphenyl-3-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-78-6P, 3-[2-Oxo-5-(2-trifluoromethylphenoxymethyl)oxazolidin-3-yl]benzamidin 540507-79-7P, N-[4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-methylnaphthalen-1-yl]acetamide 540507-80-0P, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-bis(3-methylbutyl)benzamide 540507-81-1P, 3-[5-(2-Methoxy-4-propionylphenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-82-2P, 4-[5-(2-Acetyl-4-bromophenoxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-83-3P, 3-[5-(Isoquinolin-5-yloxymethyl)-2-oxooxazolidin-3-yl]benzamidin 540507-84-4P 540507-85-5P 540507-86-6P 540507-87-7P 540507-88-8P 540507-89-9P 540507-90-2P 540507-91-3P 540507-92-4P 540507-93-5P 540507-94-6P 540507-95-7P 540507-96-8P 540507-97-9P 540507-98-0P 540507-99-1P 540508-00-7P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide 540508-01-8P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenyl)benzamide 540508-02-9P 540508-03-0P 540508-04-1P 540508-05-2P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxybenzyl)benzamide 540508-06-3P, N,N-Dibutyl-3-[3-(3-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide 540508-07-4P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dipropylbenzamide 540508-08-5P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide 540508-11-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate 540508-12-1P, N-Butyl-3-[3-(4-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide Acetate 540508-13-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-diethylbenzamide Acetate 540508-14-3P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dipropylbenzamide Acetate 540508-15-4P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dibutylbenzamide Acetate 540508-16-5P 540508-17-6P 540508-18-7P 540508-19-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-cycloheXylbenzamide Acetate 540508-20-1P, N-Benzyl-3-[3-(4-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide Acetate 540508-21-2P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-ethylbenzamide Acetate 540508-22-3P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-propylbenzamide Acetate 540508-23-4P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-fluorobenzyl)benzamide Acetate 540508-24-5P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-fluorobenzyl)benzamide Acetate 540508-25-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methylbenzyl)benzamide Acetate 540508-27-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxybenzyl)benzamide Acetate 540508-29-0P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxybenzyl)benzamide Acetate 540508-31-4P 540508-32-5P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenethylbenzamide Acetate 540508-33-6P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxyphenethyl)benzamide Acetate 540508-34-7P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-

(3,4-dimethoxyphenethyl)benzamide Acetate 540508-36-9P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenethyl)benzamide Acetate 540508-38-1P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-fluorophenyl)benzamide Acetate 540508-40-5P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methylphenyl)benzamide Acetate 540508-42-7P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxyphenyl)benzamide Formate 540508-44-9P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide Formate 540508-46-1P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3,4,5-trimethoxyphenyl)benzamide Formate 540508-48-3P 540508-51-8P, 3-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenyl)benzamide Formate 540508-56-3P 540508-58-5P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide Acetate 540508-60-9P 540508-61-0P 540508-64-3P 540508-66-5P 540508-67-6P 540508-68-7P 540508-69-8P 540508-70-1P 540508-71-2P 540508-72-3P 540508-73-4P, N-[4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide Acetate ***540508-74-5P***, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate 540508-76-7P 540508-77-8P 540508-78-9P 540508-79-0P 540508-80-3P 540508-81-4P 540508-82-5P 540508-83-6P 540508-84-7P 540508-85-8P 540508-86-9P 540508-87-0P 540508-88-1P 540508-89-2P 540508-90-5P 540508-91-6P 540508-92-7P 540508-93-8P 540508-94-9P 540508-95-0P 540508-96-1P 540508-97-2P 540508-98-3P 540508-99-4P 540509-00-0P 540509-01-1P 540509-03-3P, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-bis(3-methylbutyl)benzamide Acetate 540509-04-4P, N-[4-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-methylnaphthalen-1-yl]acetamide Acetate 540509-05-5P 540509-06-6P 540509-07-7P 540509-08-8P 540509-09-9P, N-[2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide Acetate 540509-11-3P 540509-12-4P 540509-13-5P 540509-14-6P 540509-15-7P 540509-16-8P 540509-17-9P 540509-18-0P 540509-19-1P 540509-21-5P 540509-22-6P 540509-23-7P 540509-24-8P ***540509-25-9P***, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate 540509-26-0P 540509-27-1P 540509-29-3P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT 540509-31-7P 540509-32-8P 540509-36-2P 540509-38-4P, N-[4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide Acetate 540509-40-8P 540509-42-0P 540509-44-2P 540509-46-4P 540509-48-6P, N-[2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]phenyl]acetamide Acetate 540509-51-1P 540509-52-2P 540509-54-4P 540509-56-6P 540509-57-7P 540509-58-8P 540509-59-9P 540509-60-2P 540509-61-3P 540509-62-4P, N-[4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-3-methylnaphthalen-1-yl]acetamide Acetate 540509-63-5P, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-bis(3-methylbutyl)benzamide Acetate 540509-64-6P 540509-65-7P 540509-66-8P 540509-68-0P 540509-69-1P 540509-70-4P 540509-71-5P 540509-72-6P 540509-73-7P 540509-75-9P 540509-76-0P 540509-77-1P 540509-78-2P 540509-79-3P 540509-80-6P, 4-[2-Oxo-5-(isoquinolin-5-yloxymethyl)oxazolidin-3-yl]benzamidine DiAcetate 540509-81-7P 540509-82-8P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-

phenylbenzamide Acetate 540509-83-9P 540509-84-0P 540509-85-1P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dimethylbenzamide Acetate 540509-87-3P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(4-methoxyphenyl)benzamide Acetate 540509-88-4P 540509-89-5P 540509-91-9P 540509-93-1P, 3-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-(3-methoxybenzyl)benzamide Acetate 540509-94-2P, N,N-Dibutyl-3-[3-(3-carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]benzamide Acetate 540509-96-4P 540509-97-5P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N,N-dipropylbenzamide Acetate 540509-98-6P, 4-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT 83281-56-5P 540508-09-6P 540508-10-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT 149565-66-2, Protease M
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT 55-81-2, 4-Methoxyphenethylamine 62-53-3, Phenylamine, reactions 64-04-0, Phenethylamine 70-70-2, 1-(4-Hydroxyphenyl)propan-1-one 75-04-7, Ethylamine, reactions 87-17-2, 2-Hydroxy-N-phenylbenzamide 90-15-3, Naphthalen-1-ol 90-43-7, Biphenyl-2-ol 92-69-3, Biphenyl-4-ol 96-50-4, Thiazol-2-ylamine 98-17-9, 3-Trifluoromethylphenol 98-54-4, 4-tert-Butylphenol 100-46-9, Benzylamine, reactions 100-82-3, 3-FluoroBenzylamine 102-29-4 103-90-2, N-4-(Hydroxyphenyl)acetamide 104-84-7, 4-MethylBenzylamine 104-94-9, 4-Methoxyphenylamine 106-49-0, 4-Methylphenylamine, reactions 107-10-8, Propylamine, reactions 108-91-8, Cyclohexylamine, reactions 109-73-9, n-Butylamine, reactions 109-89-7, N,N-Diethylamine, reactions 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-92-2, N,N-Di-n-butylamine 118-61-6, 2-Hydroxybenzoic acid ethyl ester 118-93-4, 1-(2-Hydroxyphenyl)ethanone 119-36-8, 2-Hydroxybenzoic acid methyl ester 120-20-7, 3,4-Dimethoxyphenethylamine 120-32-1, 2-Benzyl-4-chlorophenol 120-47-8, 4-Hydroxybenzoic acid ethyl ester 121-71-1, 3-Acetylphenol 123-75-1, Pyrrolidine, reactions 124-40-3, Dimethylamine, reactions 135-19-3, Naphthalen-2-ol, reactions 140-75-0, 4-FluoroBenzylamine 142-84-7, N,N-Dipropylamine 148-24-3, Quinolin-8-ol, reactions 371-40-4, 4-Fluorophenylamine 444-30-4, 2-Trifluoromethylphenol 487-48-9, 2-Hydroxy-N-acetylbenzamide 498-02-2, 1-(4-Hydroxy-3-methoxyphenyl)ethanone 523-68-2, N-(4-Hydroxy-3-methylnaphthalen-1-yl)acetamide 533-31-3, Benzo[1,3]dioxol-5-ol 536-90-3, 3-Methoxyphenylamine 578-67-6, Quinolin-5-ol 580-16-5, Quinolin-6-ol 580-51-8, Biphenyl-3-ol 614-80-2, N-(2-Hydroxyphenyl)acetamide 713-68-8, 3-Phenoxyphenol 828-27-3, 4-Trifluoromethoxyphenol 831-82-3, 4-Phenoxyphenol 1131-60-8, 4-Cyclohexylphenol 1450-75-5, 1-(5-Bromo-2-hydroxyphenyl)ethanone 1778-08-1, 2-Hydroxy-N,N-dimethylbenzamide 1835-14-9, 1-(4-Hydroxy-3-methoxyphenyl)propan-1-one 1953-54-4, 1H-Indol-5-ol 2039-67-0, 3-Methoxyphenethylamine 2380-86-1, 1H-Indol-6-ol 2393-23-9, 4-Methoxybenzylamine 2439-04-5,

Isoquinolin-5-ol 5060-52-6 5060-82-2, 7-Methoxynaphthalen-2-ol 5071-96-5, 3-MethoxyBenzylamine 5111-66-0, 6-Methoxynaphthalen-2-ol 5402-37-9, 4-Indan-1-ylphenol 5446-02-6, 2-Hydroxy-4-methoxybenzoic acid methyl ester 5597-50-2, 3-(4-Hydroxyphenyl)propionic acid methyl ester 5614-78-8, Chroman-6-ol 6746-81-2, Glycidyltosylate 10041-02-8, 4-Imidazol-1-ylphenol 14121-97-2, 4-Hydroxy-N-phenylbenzamide 15504-60-6, (3-Hydroxyphenyl)piperidin-1-ylmethanone 15789-03-4, 3-Hydroxy-N,N-dimethylbenzamide 15789-05-6, (3-Hydroxyphenyl)morpholin-4-ylmethanone 17138-28-2 17826-14-1, 5-Hydroxy-2-methyl-1-propyl-1H-indol-3-carboxylic acid ethyl ester 18137-25-2, (4-Hydroxyphenyl)morpholin-4-ylmethanone 18979-50-5, 4-Propoxyphenol 19438-10-9, 3-Hydroxybenzoic acid methyl ester 22479-95-4 24313-88-0, 3,4,5-Trimethoxyphenylamine 27292-50-8, 3-Piperidin-1-ylphenol 27559-45-1, 3-Hydroxy-N-phenylbenzamide 35320-67-3, 2-Methyl-1H-indol-4-ol 41536-44-1, 2-Morpholin-4-ylphenol 58547-68-5, (4-Hydroxyphenyl)piperidin-1-ylmethanone 65195-20-2, 2-Piperidin-1-ylphenol 67914-60-7, 1-[4-(4-Hydroxyphenyl)piperazin-1-yl]ethanone 75999-00-7, 4-(1,3,5-Trimethyl-1H-pyrazol-4-ylmethyl)phenol 77802-89-2, 2,4-Dichloro-6-piperidin-1-ylmethylphenol 80917-39-1, (3-Hydroxyphenyl)pyrrolidin-1-ylmethanone 83167-91-3, 4-(4-Propylcyclohexyl)phenol 83281-53-2 93919-56-3, 4-Trifluoromethoxybenzylamine 101744-90-5, N,N-Bis(3-methylbutyl)benzamide 105211-78-7, 4-Hydroxy-3-propylbenzoic acid methyl ester 194225-11-1, 4-Hydroxy-N,N-dipropylbenzamide 222544-30-1 227326-99-0 301172-82-7, 3-Hydroxy-N,N-dibutylbenzamide 415928-53-9, 2-Methoxy-4-morpholin-4-ylmethylphenol 478929-28-1, (4-Hydroxyphenyl)pyrrolidin-1-ylmethanone 540508-54-1, 4-(5-Methylpyridin-2-yl)phenol 540508-75-6, 4-(2-p-Tolylethyl)phenol 540509-02-2, 2-[Bis(3-methylbutyl)amino]-1-(2-hydroxyphenyl)ethanone 540509-10-2 540509-20-4, 5-Methyl-2-(3-phenylpropyl)phenol 540509-74-8, 4-(4-Methyl-4H-[1,2,4]triazol-3-yl)phenol 540509-86-2, 3-Hydroxy-N-(4-methoxyphenyl)benzamide 540509-92-0, 3-Hydroxy-N-(3-methoxybenzyl)benzamide

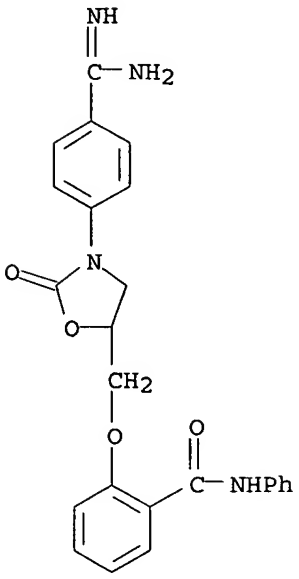
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

IT ***540506-32-9P***, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide ***540507-31-1P***, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide ***540508-74-5P***, 2-[3-(4-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate ***540509-25-9P***, 2-[3-(3-Carbamimidoylphenyl)-2-oxooxazolidin-5-ylmethoxy]-N-phenylbenzamide Acetate

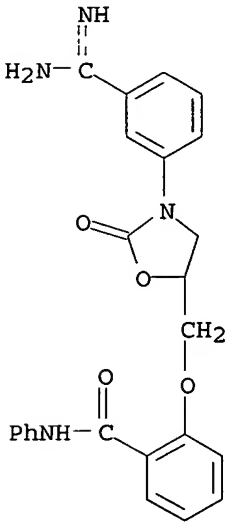
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of phenyloxazolidinones as protease M inhibitors for the treatment of ***tumor*** illnesses and neurodegenerative diseases)

RN 540506-32-9 HCAPLUS

CN Benzamide, 2-[[3-[4-(aminoiminomethyl)phenyl]-2-oxo-5-oxazolidinyl]methoxy]-N-phenyl- (9CI) (CA INDEX NAME)



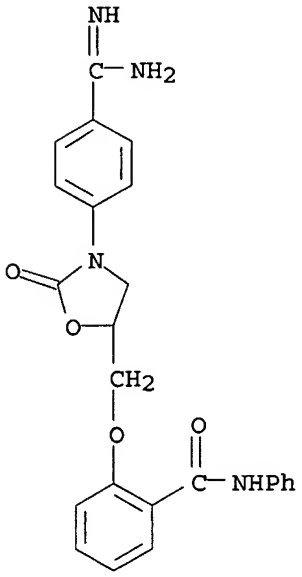
RN 540507-31-1 HCAPLUS
CN Benzamide, 2-[[3-[3-(aminoiminomethyl)phenyl]-2-oxo-5-oxazolidinyl]methoxy]-N-phenyl- (9CI) (CA INDEX NAME)



RN 540508-74-5 HCAPLUS
CN Benzamide, 2-[[3-[4-(aminoiminomethyl)phenyl]-2-oxo-5-oxazolidinyl]methoxy]-N-phenyl-, monoacetate (9CI) (CA INDEX NAME)

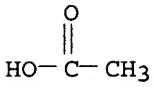
CM 1

CRN 540506-32-9
CMF C24 H22 N4 O4



CM 2

CRN 64-19-7
CMF C2 H4 O2



RN 540509-25-9 HCAPLUS
CN Benzamide, 2-[[3-[3-(aminoiminomethyl)phenyl]-2-oxo-5-oxazolidinyl]methoxy]-N-phenyl-, monoacetate (9CI) (CA INDEX NAME)

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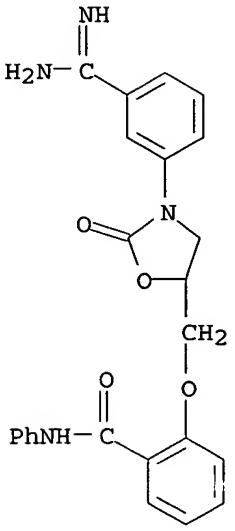

CM 2

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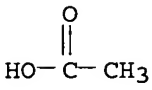


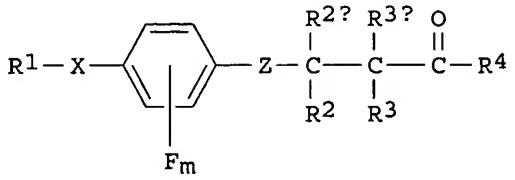
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 3 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:255113 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 138:271392
TITLE: Benzenebutyric acids and their derivatives as inhibitors of matrix metalloproteinases
INVENTOR(S): Purchase, Claude Forsey, Jr.; Roth, Bruce David; White, Andrew David
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: U.S., 38 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6541521	B1	20030401	US 1999-351549	19990712 <--
US 2002161050	A1	20021031	US 2001-23288	20011217 <--
US 6624196	B2	20030923		

PRIORITY APPLN. INFO.: US 1999-351549 A3 19990712 <--

OTHER SOURCE(S): MARPAT 138:271392
GI



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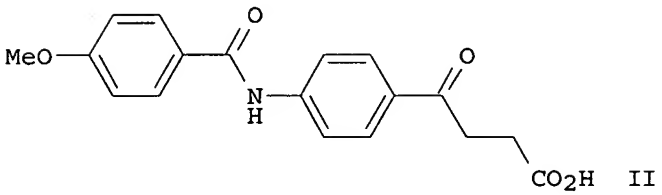

II

AB Title compds. I and their isomers and pharmaceutically acceptable salts are disclosed [wherein: R1 = H, (cyclo)alkyl, (hetero)aryl, (hetero)arylalkyl, heterocyclyl(alkyl); X = (un)substituted COCH2, CONH, NHCO, COO, OCO, CO, CH(OH), C(:NH)NH, OCOO, OCONH, NHCOO, NHCONH, C(:S)NH, NHC(:S), C(:S)O, OC(:S), OC(:S)O, OC(:S)NH, NHC(:S)O, NHC(:S)NH; m = 0-4; Z = CO, (un)substituted C(:NOH) or CH(OH), CHF, CF2; R2, R2a, R3, R3a = (independently) H, F, R5, (un)substituted -alkyl-R5, (un)substituted -NHCO-alkyl or -NH-alkyl; R4 = SH, OH, alkoxy, aralkoxy, cycloalkoxy, etc.; R5 = H, (hetero)aryl, heterocyclyl, phthalimido, 2,3-naphthylimido, indol-3-yl, imidazol-4-yl, 2-, 3-, or 4-pyridyl, 2,4-dioxo-1,5,5-trimethylimidazolidin-3-yl,or an (un)natural amino acid sidechain]. Novel compds. and derivs. are described, as well as methods for their preparation, and pharmaceutical compns. containing them. Compds. I are useful as inhibitors of matrix metalloproteinases (MMPs), particularly gelatinase A (MMP-2), collagenase-3 (MMP-13), and stromelysin-1 (MMP-3). I are thereby useful for the treatment of multiple sclerosis, atherosclerotic plaque rupture, aortic aneurysm, heart failure, left ventricular dilation, restenosis, periodontal disease, corneal ulceration, treatment of burns, decubital ulcers, wound healing, ***cancer***, inflammation, pain, arthritis, osteoporosis, renal disease, or other autoimmune or inflammatory disorders dependent upon tissue invasion by leukocytes or other activated migrating cells, acute and chronic neurodegenerative disorders including stroke, head trauma, spinal cord injury, Alzheimer's disease, amyotrophic lateral sclerosis, cerebral amyloid angiopathy, ***AIDS***, Parkinson's disease, Huntington's disease, prion diseases, myasthenia gravis, and Duchenne's muscular dystrophy. A total of 36 compds. I were prepared and tested against the 3 aforementioned MMPs. For instance, Friedel-Crafts acylation of acetanilide by succinic anhydride in DMF in the presence of AlCl3 gave 4-(AcNH)C6H4COCH2CH2CO2H, which was deacetylated with aqueous HCl and then treated with Me3SiCH:N2 in PhMe/MeOH mixture to give 4-H2NC6H4COCH2CH2CO2Me. Amidation of this amine with 4-MeOC6H4COCl using 4-morpholinomethyl polystyrene resin gave title compound II. Compound II inhibited MMP catalytic domains (CD) in vitro as follows (IC50): MMP-2CD 0.07, MMP-3CD 0.34, and MMP-13CD 9.8 μM.

IC ICM A61K031-195
ICS C07C207-00; C07C229-00
INCL 514567000; 562435000; 562438000; 562455000
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
IT Analgesics
Anti-***AIDS*** agents
Anti-Alzheimer's agents
Anti-inflammatory agents
Antiarthritics
Antiparkinsonian agents
Antitumor agents
Cardiovascular agents
Human
Immunosuppressants
Wound healing promoters
(preparation of benzenebutyric acids and derivs. as inhibitors of matrix metalloproteinases)
IT ***AIDS (disease)***
Alzheimer's disease
Arthritis
Autoimmune disease
Burn
Inflammation
Kidney, disease
Multiple sclerosis
Myasthenia gravis
Neoplasm
Osteoporosis
Pain
Parkinson's disease
Periodontium, disease
Prion diseases
Wound
(treatment of; preparation of benzenebutyric acids and derivs. as inhibitors of matrix metalloproteinases)
IT 42811-23-4P, 4-Oxo-4-[4-(3-phenylureido)phenyl]butyric acid 42811-24-5P, 4-[4-[3-(4-Chlorophenyl)ureido]phenyl]-4-oxobutyric acid 63471-86-3P, 4-[4-[(4-Chlorobenzoyl)amino]phenyl]-4-oxobutyric acid 474016-23-4P, 4-Hydroxyimino-4-[4-[(4-methylbenzoyl)amino]phenyl]butyric acid 474016-29-0P, 4-Oxo-4-(4-pentanoylaminophenyl)butyric acid 474016-34-7P, 4-[4-[(3-Fluorobenzoyl)amino]phenyl]-4-oxobutyric acid 474016-39-2P, 4-[4-[(2-Fluorobenzoyl)amino]phenyl]-4-oxobutyric acid 474016-44-9P, 4-[4-[(4-Fluorobenzoyl)amino]phenyl]-4-oxobutyric acid 474016-48-3P, 4-[4-[(Cyclohexanecarbonyl)amino]phenyl]-4-oxobutyric acid 474016-52-9P, 4-[4-[(Pyridin-3-ylcarbonyl)amino]phenyl]-4-oxobutyric acid 474016-57-4P, 4-[4-(Nonanoylamino)phenyl]-4-oxobutyric acid 474016-62-1P, 4-[4-(Octanoylamino)phenyl]-4-oxobutyric acid 474016-68-7P, 4-Oxo-4-[4-(propionylamino)phenyl]butyric acid 474016-73-4P, 4-[4-[(3-Methoxybenzoyl)amino]phenyl]-4-oxobutyric acid 474016-78-9P, 4-[4-[(2,4-Dichlorobenzoyl)amino]phenyl]-4-oxobutyric acid 474016-84-7P, 4-[4-[[4-(4-Bromophenyl)butyryl]amino]phenyl]-4-oxobutyric acid 474016-89-2P, 4-[4-(Heptanoylamino)phenyl]-4-oxobutyric acid 474016-93-8P, 4-[4-[(4-Ethylbenzoyl)amino]phenyl]-4-oxobutyric acid 474016-99-4P, 4-[4-[(4-Butoxybenzoyl)amino]phenyl]-4-oxobutyric acid 474017-03-3P, 4-[4-[(4-Chloro-3-nitrobenzoyl)amino]phenyl]-4-oxobutyric acid 474017-08-8P, 4-[4-(Cinnamoylamino)phenyl]-4-oxobutyric acid 474017-12-4P, 4-[4-[(4-Bromobenzoyl)amino]phenyl]-4-oxobutyric acid 474017-15-7P, 4-[4-[(3-Nitrobenzoyl)amino]phenyl]-4-oxobutyric acid

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RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzenebutyric acids and derivs. as inhibitors of matrix metalloproteinases)

IT ***474017-28-2P***, 4-[4-[(2-Methoxybenzoyl)amino]phenyl]-4-oxobutyric acid ***474018-03-6P***, 4-[4-[(2,4-Dimethoxybenzoyl)amino]phenyl]-4-oxobutyric acid ***474018-07-0P***, 4-[4-[(2,5-Dimethoxybenzoyl)amino]phenyl]-4-oxobutyric acid ***474020-23-0P***, 4-Hydroxyimino-4-[4-[(2-methoxybenzoyl)amino]phenyl]butyric acid ***474020-32-1P***, 4-[4-[(2,4-Dimethoxybenzoyl)amino]phenyl]-4-(hydroxyimino)butyric acid ***474020-34-3P***, 4-[4-[(2,5-

Dimethoxybenzoyl)amino]phenyl]-4-(hydroxyimino)butyric acid
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of benzenebutyric acids and derivs. as inhibitors of matrix metalloproteinases)

RN 474017-28-2 HCAPLUS
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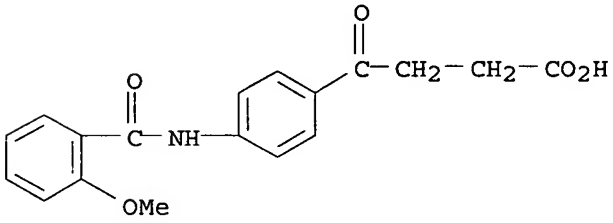

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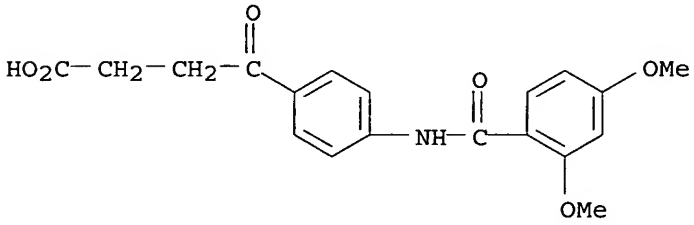

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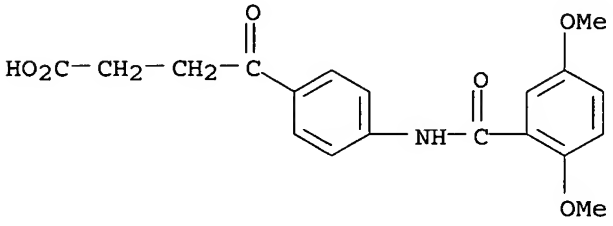

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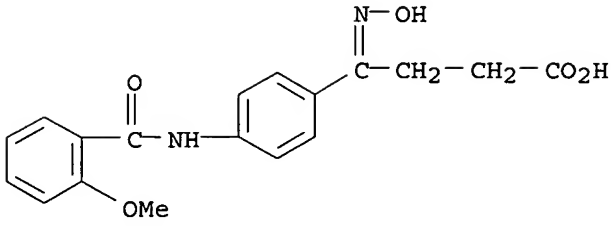

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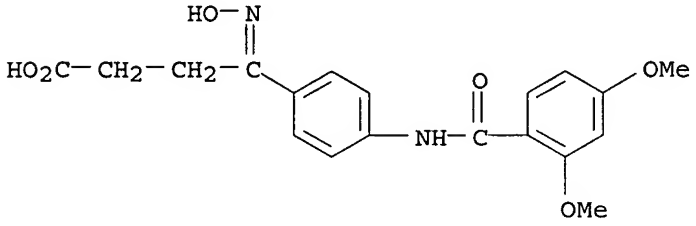

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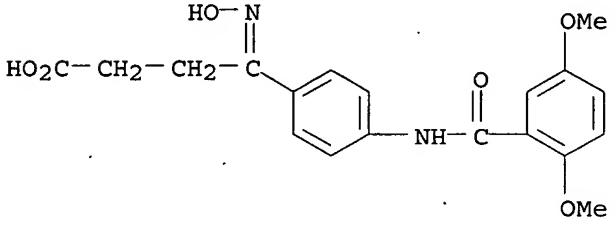

REFERENCE COUNT: 93 THERE ARE 93 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 4 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:173600 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 138:221591
TITLE: Preparation of new substituted 4-(4-piperidinyl)morpholines as modulators of chemokine receptor activity
INVENTOR(S): Gustafsson, Joergen; Hossain, Nafizal; Nilsson, Stinabritt
PATENT ASSIGNEE(S): Astrazeneca A.B., Swed.
SOURCE: PCT Int. Appl., 50 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003018576	A1	20030306	WO 2002-SE1487	20020821 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
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AT 315563	E	20060215	AT 2002-760960	20020821 <--
US 2004204408	A1	20041014	US 2004-486505	20040211 <--
PRIORITY APPLN. INFO.:			GB 2001-20461 A	20010822 <--
			WO 2002-SE1487 W	20020821

OTHER SOURCE(S): MARPAT 138:221591
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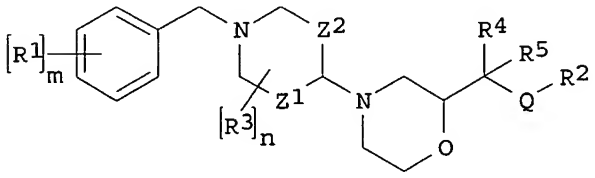


I

AB The title compds. [I; m = 0-3; R1 = halo, CN, NO2, etc.; Z1 = a bond, (CH2)q (q = 1-2); Z2 = a bond, CH2, with the proviso that Z1 and Z2 do not both simultaneously represent a bond; Q = O, S, CH2, NH; R2 = (un)substituted unsatd. 5-10 membered ring system which may comprise at least one ring heteroatom; n = 0-2; R3 = alkyl, alkoxycarbonyl, CH2OH, CO2H; R4, R5 = H, alkyl], useful for the treatment of human diseases or conditions in which modulation of chemokine receptor activity is beneficial, were prepared E.g., a multi-step synthesis of I [R1 = 4-Cl; m = 1; R2 = 2-(MeCONH)C6H4; n = 0; R4, R5 = H; Q = O; Z1, Z2 = CH2], starting from 4-(tert-butoxycarbonyl)-2-morpholinecarboxylic acid, was given.

IC ICM C07D413-04
ICS C07D413-14; A61K031-5377; A61P011-00; A61P019-00; A61P031-00; A61P037-00

CC 28-13 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST piperidinyl morpholine prepn chemokine MIP1alpha receptor modulator ***antiasthmatic*** antiinflammatory; macrophage inflammatory protein 1alpha chemokine modulator piperidinyl morpholine prepn

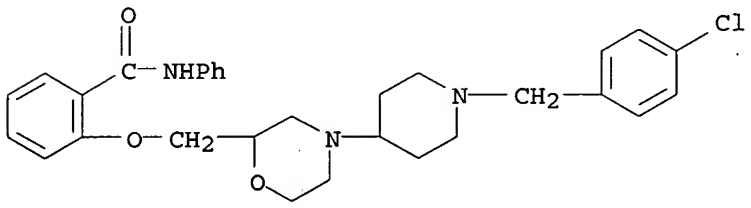
IT Anti-inflammatory agents
Antiasthmatics
Antirheumatic agents
Human
(preparation of new substituted 4-(4-piperidinyl)morpholines as modulators of chemokine receptor activity)

IT ***Asthma***
Inflammation
Multiple sclerosis
Respiratory system, disease
Rheumatoid arthritis
(treatment of; preparation of new substituted 4-(4-piperidinyl)morpholines as modulators of chemokine receptor activity)

IT 500789-10-6P 500789-12-8P 500789-13-9P 500789-14-0P 500789-15-1P
500789-16-2P 500789-17-3P 500789-18-4P 500789-19-5P 500789-20-8P
500789-21-9P 500789-22-0P ***500789-23-1P*** 500789-24-2P
500789-25-3P 500789-26-4P 500789-27-5P 500789-28-6P 500789-29-7P
500789-30-0P 500789-31-1P 500789-32-2P 500789-33-3P 500789-34-4P
500789-35-5P 500789-36-6P 500789-37-7P 500789-38-8P 500789-39-9P
500789-40-2P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new substituted 4-(4-piperidinyl)morpholines as modulators of chemokine receptor activity)

IT ***500789-23-1P***
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new substituted 4-(4-piperidinyl)morpholines as modulators of chemokine receptor activity)

RN 500789-23-1 HCAPLUS
CN Benzamide, 2-[[4-[1-[(4-chlorophenyl)methyl]-4-piperidinyl]-2-morpholinyl]methoxy]-N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

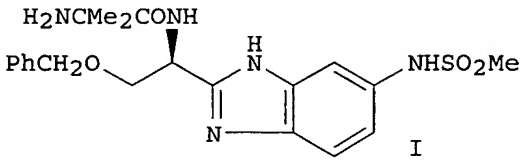
L101 ANSWER 5 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:150554 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 138:188073
TITLE: Preparation of dipeptide heterocyclic aromatic compounds as growth hormone secretagogues
INVENTOR(S): Tino, Joseph A.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: U.S., 157 pp., Cont.-in-part of U.S. Ser. No. 506,749, abandoned.
CODEN: USXXAM

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6525203	B1	20030225	US 2000-662448	20000914 <--
US 6518292	B1	20030211	US 2000-506749	20000218 <--
ZA 2001006854	A	20021120	ZA 2001-6854	20010820 <--
US 6660760	B1	20031209	US 2002-282182	20021028 <--
US 2004002525	A1	20040101	US 2002-281818	20021028 <--
US 6969727	B2	20051129		
US 2004029935	A1	20040212	US 2002-281649	20021028 <--
US 6908938	B2	20050621		
US 2004072881	A1	20040415	US 2002-281848	20021028 <--
US 7053110	B2	20060530		

PRIORITY APPLN. INFO.: US 1999-124131P P 19990312 <--
US 1999-154919P P 19990921 <--
US 2000-506749 A2 20000218 <--

OTHER SOURCE(S): MARPAT 138:188073
GI



I

AB R1R1aCXaNR6COYXb [R1 = (un)substituted alkyl, (hetero)aryl(alkyl), etc.; R1a = H or (cyclo)alkyl; R6 = H, (cyclo)alkyl, alkenyl, aryl; Xa = substituted 2-benzoxazolyl, 2-benzothiazolyl, or 2-benzimidazolyl; Xb = (di)(alkyl)amino, (un)substituted imidazolyl; Y = phenylene, (phenylene-interrupted)alkylene, (un)substituted alkylene, aza- or oxaalkylene, or alkenylene] were prepared as growth hormone production and/or release stimulants. Thus, dipeptide benzimidazole derivative I (Boc = tert-butoxycarbonyl) was prepared by a multistep procedure starting from Boc-D-Ser(CH2Ph)-OH, 4-nitro-o-phenylenediamine, Boc-methylalanine, and MeSO2Cl.

IC ICM C07D401-12
ICS A01K031-11

INCL 548125000; 514367000; 514375000; 548180000; 548217000; 548309700

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 2, 28

IT ***AIDS (disease)***
Human immunodeficiency virus 1
(***HIV*** wasting syndrome; preparation of dipeptide heterocyclic aromatic compds. as growth hormone secretagogues)

IT 295336-38-8P 295336-39-9P 295336-40-2P 295336-41-3P 295336-42-4P
295336-43-5P 295336-44-6P 295336-45-7P 295336-46-8P 295336-47-9P
295336-48-0P 295336-49-1P 295336-50-4P 295336-51-5P 295336-52-6P
295336-53-7P 295336-54-8P 295336-55-9P 295336-56-0P 295336-57-1P
295336-58-2P 295336-59-3P 295336-60-6P 295336-61-7P 295336-62-8P
295336-63-9P 295336-64-0P 295336-65-1P ***295336-66-2P***

295336-67-3P 295336-68-4P 295336-69-5P 295336-70-8P 295336-72-0P
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295336-78-6P 295336-79-7P 295336-80-0P 295336-81-1P 295336-82-2P
295336-83-3P 295336-84-4P 295336-85-5P 295336-86-6P 295336-87-7P
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498576-51-5P 498576-52-6P 498576-53-7P 498577-07-4P

RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dipeptide heterocyclic aromatic compds. as growth hormone secretagogues)

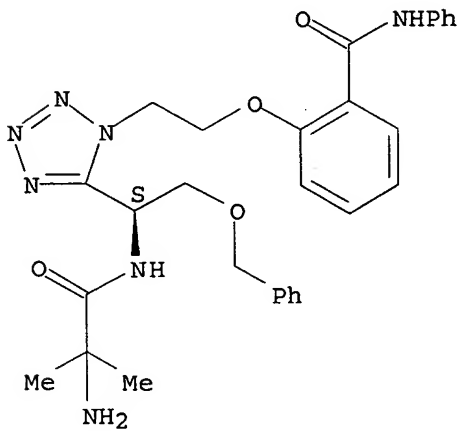
IT ***295336-66-2P***

RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dipeptide heterocyclic aromatic compds. as growth hormone secretagogues)

RN 295336-66-2 HCAPLUS

CN Benzamide, 2-[2-[5-[(1S)-1-[(2-amino-2-methyl-1-oxopropyl)amino]-2-(phenylmethoxy)ethyl]-1H-tetrazol-1-yl]ethoxy]-N-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

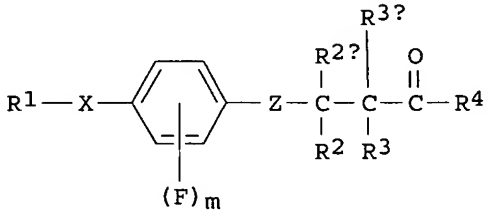


REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

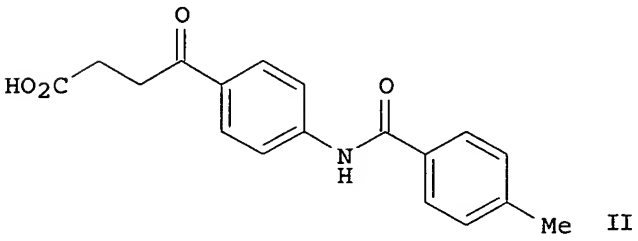
L101 ANSWER 6 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:833521 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 137:337683
TITLE: Preparation of benzenebutyric acids as inhibitors of matrix metalloproteinases
INVENTOR(S): Purchase, Claude Forsey; Roth, Bruce David; White, Andrew David
PATENT ASSIGNEE(S): Warner-Lambert Company, USA
SOURCE: U.S. Pat. Appl. Publ., 43 pp., Division of U. S. Ser. No. 351,549.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002161050	A1	20021031	US 2001-23288	20011217 <--
US 6624196	B2	20030923		
US 6541521	B1	20030401	US 1999-351549	19990712 <--
PRIORITY APPLN. INFO.:			US 1999-351549 A3	19990712 <--
OTHER SOURCE(S):	MARPAT 137:337683			

GI



I



II

AB The title compds. with general formula of I [wherein R1 = H, (cyclo)alkyl, (hetero)aryl, (hetero)arylalkyl, or heterocyclyl(alkyl); R2, R2a, R3, and R3a = independently H, F, R5, NR7CO-alkyl, alkanoyl(oxy), alkoxycarbonyl, alkanoylthio, NR7-alkyl, alkylsulfinyl, alkylsulfonyl(amino), CN, CF3, or (un)substituted alkyl-R5; R5 = H, (hetero)aryl, heterocyclyl, N-naphthalimido, N-2,3-naphthylimido, indol-3-yl, imidazol-4-yl, pyridyl,

2,4-dioxo-1,5,5-trimethylimidazolidin-3-yl, or a side chain of an (un)naturally occurring amino acid; R4 = SH, OR4a, or NHOR4a; R4a = H, (aryl)alkyl, cycloalkyl, or aryloxymethyl; X = COCH2, CONR6, NR6CO, CO2, OCO, CO, CH(OH), C(=NH)NR6, OCO2, OCONR6, NR6CO2, NR6CONR6a, CSNR6, NR6CS, CSO, OCS, OCSO, OCSNR6, NR6CSO, or NR6CSNR6a; R6 and R6a = independently H or CH3; or R1 and R6 together form a ring containing (un)substituted 4-7 carbons, etc.; Z = CO, CN(OR7), C(OH)R7, CHF, or CF2; R7 = H or alkyl; m = 0-4; or isomers and pharmaceutically acceptable salts thereof] where prepared as inhibitors of matrix metalloproteinases (MMP), particularly gelatinase A, collagenase-3, and stromelysin-1. For example, reaction of acetanilide and succinic anhydride in DMF in the presence of AlCl3 gave 4-(4-acetylaminophenyl)-4-oxobutyric acid. The above compound was treated with 1.0 M aqueous HCl, followed by 50% weight/weight aqueous NaOH, and again by 1.0 M aqueous HCl to give 4-(4-aminophenyl)-4-oxobutyric acid. Subsequent esterification, amidation, and hydrolysis of the above compound afforded 4-[4-(4-methylbenzoylamino)phenyl]-4-oxobutyric acid (II). II showed the activity vs. MMP-2CD, MMP-3CD, and MMP-13CD with IC50 values of 0.22 μM, 1.55 μM, and 5.8 μM, resp. I are useful for the treatment of multiple sclerosis, atherosclerotic plaque rupture, aortic aneurysm, heart failure, left ventricular dilation, restenosis, periodontal disease, corneal ulceration, treatment of burns, decubital ulcers, wound healing, ***cancer***, inflammation, pain, arthritis, osteoporosis, renal disease, or other autoimmune or inflammatory disorders dependent upon tissue invasion by leukocytes or other activated migrating cells, acute and chronic neurodegenerative disorders including stroke, head trauma, spinal cord injury, Alzheimer's disease, amyotrophic lateral sclerosis, cerebral amyloid angiopathy, ***AIDS***, Parkinson's disease, Huntington's disease, prion diseases, myasthenia gravis, and Duchenne's muscular dystrophy (no data).

IC ICM A61K031-192
ICS A61K031-21

INCL 514568000

CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

IT ***AIDS (disease)***
Alzheimer's disease
Analgesics
Anti-***AIDS*** agents
Anti-Alzheimer's agents
Anti-inflammatory agents
Antiarthritics
Antiparkinsonian agents
Antitumor agents
Arthritis
Atherosclerosis
Autoimmune disease
Burn
Cardiovascular agents
Human
Immunomodulators
Inflammation
Kidney, disease
Multiple sclerosis
Myasthenia gravis
Neoplasm
Nervous system agents
Osteoporosis
Pain

Parkinson's disease
Periodontium, disease
Prion diseases
Wound healing
(preparation of benzenebutyric acids as inhibitors of matrix metalloproteinases)

IT 42811-23-4P 42811-24-5P 63471-86-3P 474016-07-4P 474016-23-4P
474016-29-0P 474016-34-7P 474016-39-2P 474016-44-9P 474016-48-3P
474016-52-9P 474016-57-4P 474016-62-1P 474016-68-7P 474016-73-4P
474016-78-9P 474016-84-7P 474016-89-2P 474016-93-8P 474016-99-4P
474017-03-3P 474017-08-8P 474017-12-4P 474017-15-7P 474017-18-0P
474017-21-5P 474017-24-8P ***474017-28-2P*** 474017-34-0P
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474017-56-6P 474017-61-3P 474017-64-6P 474017-67-9P 474017-70-4P
474017-75-9P 474017-79-3P 474017-83-9P 474017-87-3P 474017-89-5P
474017-93-1P 474017-97-5P ***474018-03-6P 474018-07-0P***
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474020-73-0P 474020-74-1P 474020-76-3P 474020-78-5P 474020-80-9P
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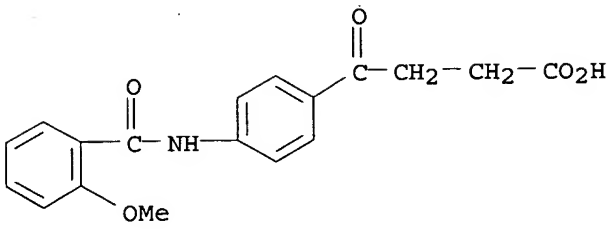
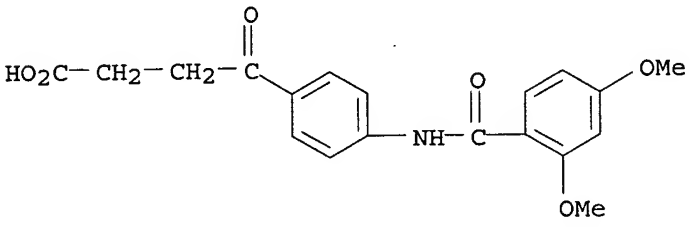
474021-10-8P 474021-12-0P 474021-14-2P 474021-15-3P 474021-17-5P
474021-19-7P 474021-20-0P 474021-23-3P 474021-24-4P 474021-26-6P
474021-28-8P 474021-30-2P 474021-32-4P 474021-34-6P 474021-36-8P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(MMP inhibitor; preparation of benzenebutyric acids as inhibitors of matrix metalloproteinases)

IT ***474017-28-2P 474018-03-6P 474018-07-0P***
474020-23-0P 474020-32-1P 474020-34-3P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(MMP inhibitor; preparation of benzenebutyric acids as inhibitors of matrix metalloproteinases)

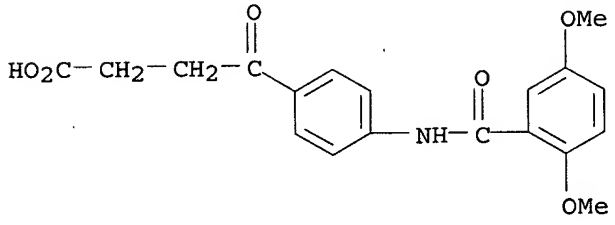
RN 474017-28-2 HCAPLUS
CN Benzenebutanoic acid, 4-[(2-methoxybenzoyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



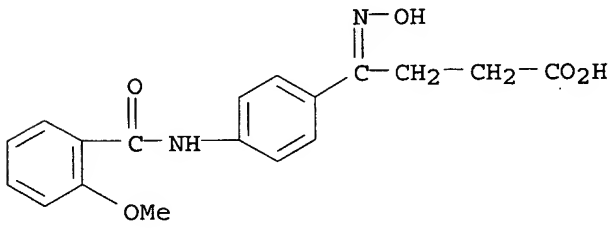
RN 474018-03-6 HCAPLUS
CN Benzenebutanoic acid, 4-[(2,4-dimethoxybenzoyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



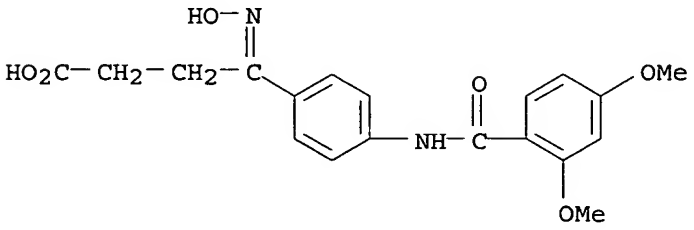
RN 474018-07-0 HCAPLUS
CN Benzenebutanoic acid, 4-[(2,5-dimethoxybenzoyl)amino]-γ-oxo- (9CI) (CA INDEX NAME)



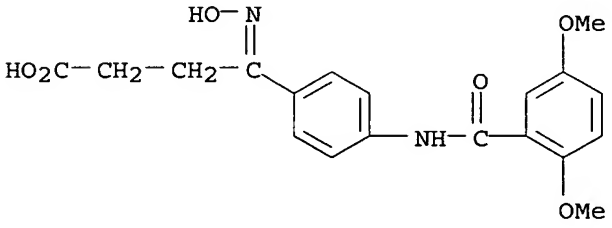
RN 474020-23-0 HCAPLUS
CN Benzenebutanoic acid, γ-(hydroxyimino)-4-[(2-methoxybenzoyl)amino]- (9CI) (CA INDEX NAME)



RN 474020-32-1 HCAPLUS
CN Benzenebutanoic acid, 4-[(2,4-dimethoxybenzoyl)amino]-γ-(hydroxyimino)- (9CI) (CA INDEX NAME)



RN 474020-34-3 HCAPLUS
CN Benzenebutanoic acid, 4-[(2,5-dimethoxybenzoyl)amino]-γ-(hydroxyimino)- (9CI) (CA INDEX NAME)



L101 ANSWER 7 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:754333 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 137:279214
TITLE: Preparation of benzoic acid derivatives as nuclear factor κB inhibitors
INVENTOR(S): Suzuki, Kenji; Nunokawa, Youichi; Ogou, Naohisa
PATENT ASSIGNEE(S): Suntory Limited, Japan; Suntory Biomedical Research Limited
SOURCE: PCT Int. Appl., 243 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

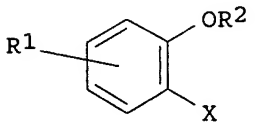
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002076918	A1	20021003	WO 2002-JP3017	20020327 <--
WO 2002076918	C1	20021031		
W: BR, CA, CN, HU, JP, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2410816	AA	20021003	CA 2002-2410816	20020327 <--
BR 2002004678	A	20030429	BR 2002-4678	20020327 <--
EP 1314712	A1	20030528	EP 2002-708696	20020327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, FI, CY, TR

US 2004122244	A1	20040624	US 2002-296810		20021127 <--
US 7064124	B2	20060620			
PRIORITY APPLN. INFO.:			JP 2001-91003	A	20010327 <--
			WO 2002-JP3017	W	20020327

OTHER SOURCE(S): MARPAT 137:279214

GI



I

AB The title compds. I [R1 = (1,4-benzoquinon-2-yl)methyl (with substituents selected from H, alkyl, etc.) (generic structure given), etc.; R2 = H, (un)substituted alkyl, etc.; X = carboxyl (which may esterified or amidated)] are prepared In an in vitro test for nuclear factor κB inhibiting activity, N-[5-(5,6-dimethoxy-3-methyl-1,4-benzoquinon-2-yl)methyl-2-hydroxybenzoyl]-4-aminobenzoic acid Et ester showed IC50 value of 3 μg/mL.

IC ICM C07C065-24
ICS C07C065-40; C07C069-157; C07C069-94; C07C235-64; C07C255-24; C07C255-63; C07C317-40; C07D295-18; C07D215-08; C07D233-02; C07D213-30; C07D213-75; C07D211-16; C07D231-12; C07D239-47

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25

IT Adenoviridae
Cytomegalovirus
Human T-lymphotropic virus 1
Human immunodeficiency virus
Simian virus 40
(gene expression inhibitor; preparation and bioeffect of benzoic acid derivs. with nuclear factor κB inhibiting activity)

IT Interleukin 1
Interleukin 2
Interleukin 6
Interleukin 8
Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(gene expression inhibitor; preparation and bioeffect of benzoic acid derivs. with nuclear factor κB inhibiting activity)

IT 464213-92-1P 464213-93-2P 464213-95-4P 464213-99-8P 464214-00-4P
464214-01-5P 464214-56-0P 464214-57-1P ***464214-59-3P***
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464215-94-9P
RL: ***PAC (Pharmacological activity)***; RCT (Reactant); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoic acid derivs. as nuclear factor κB inhibitors)

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464215-95-0P 464215-96-1P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid derivs. as nuclear factor κB inhibitors)

IT ***464214-59-3P*** ***464214-61-7P*** ***464214-63-9P***
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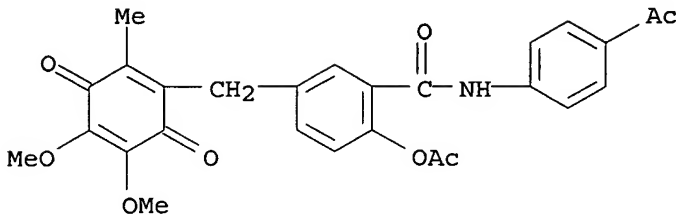
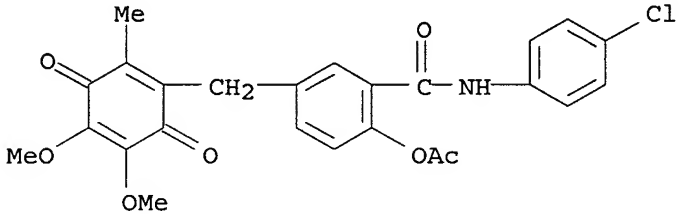
464215-08-5P ***464215-09-6P*** ***464215-11-0P***
464215-23-4P ***464215-34-7P*** ***464215-46-1P***
464215-47-2P ***464215-92-7P***
RL: ***PAC (Pharmacological activity)***; RCT (Reactant); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoic acid derivs. as nuclear factor κB inhibitors)

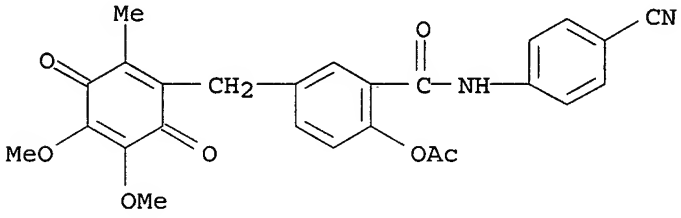
RN 464214-59-3 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-(4-acetylphenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



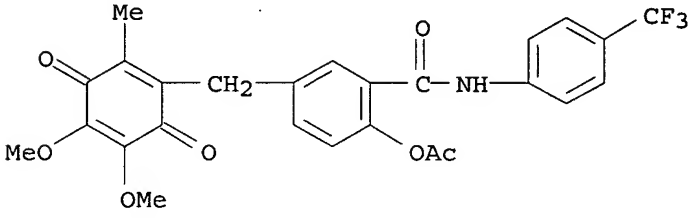
RN 464214-61-7 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-(4-chlorophenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



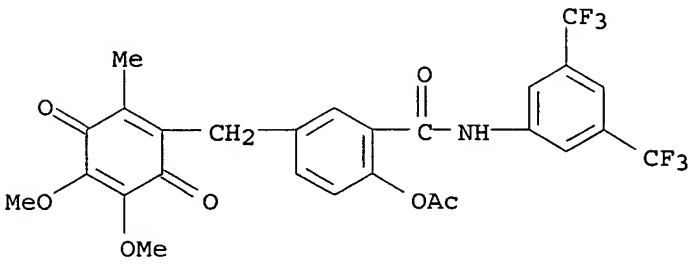
RN 464214-63-9 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-(4-cyanophenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



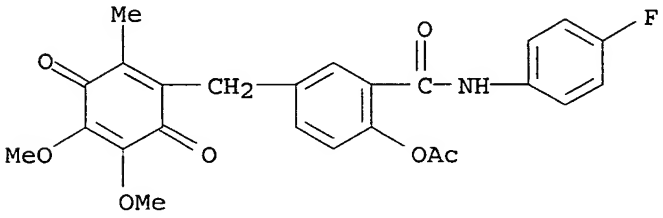
RN 464214-64-0 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



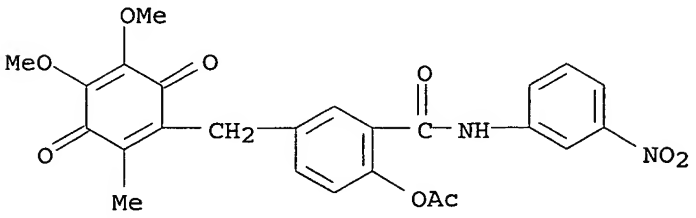
RN 464214-65-1 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-[3,5-bis(trifluoromethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



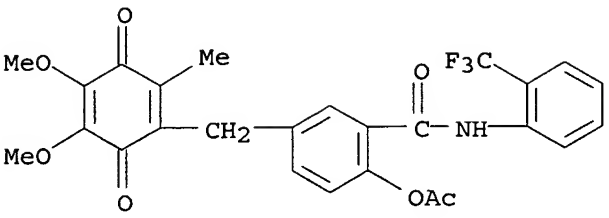
RN 464214-99-1 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



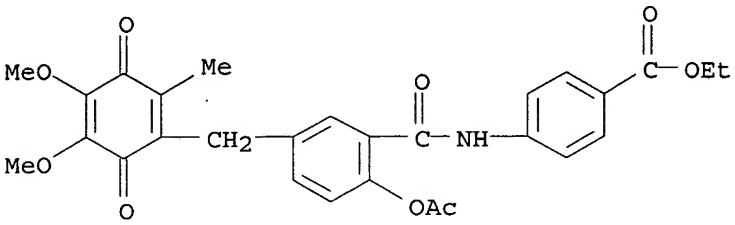
RN 464215-01-8 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



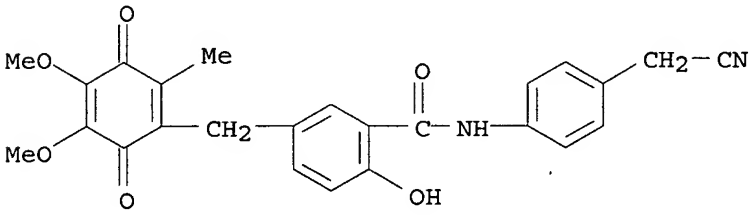
RN 464215-03-0 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



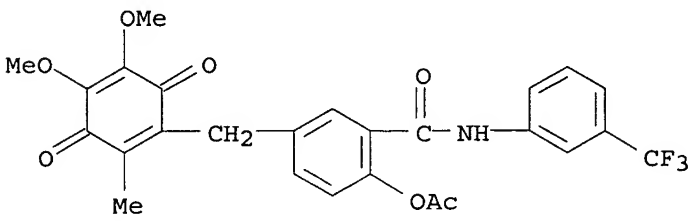
RN 464215-05-2 HCAPLUS
CN Benzoic acid, 4-[[2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



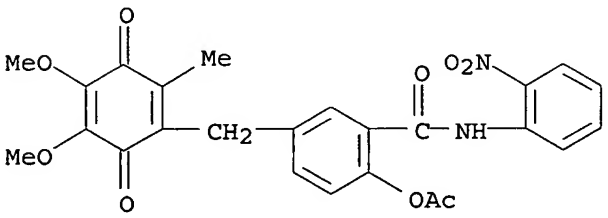
RN 464215-08-5 HCAPLUS
CN Benzamide, N-[4-(cyanomethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



RN 464215-09-6 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 464215-11-0 HCAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



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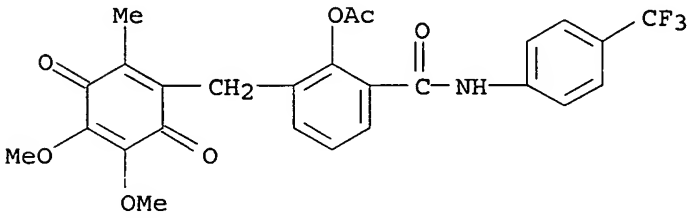
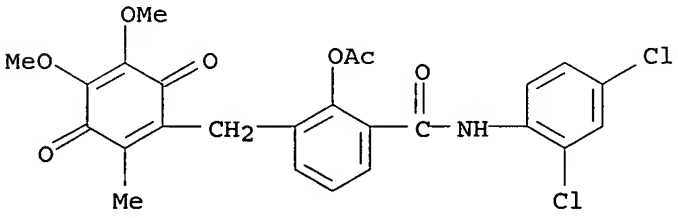
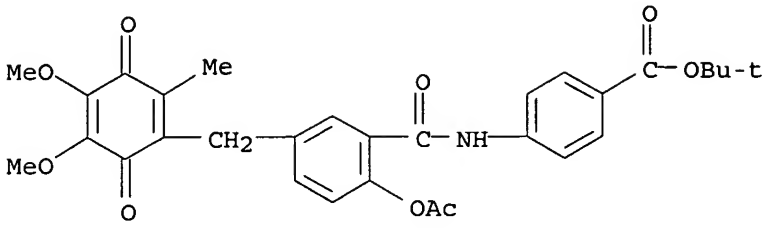
CN Benzamide, 2-(acetyloxy)-3-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



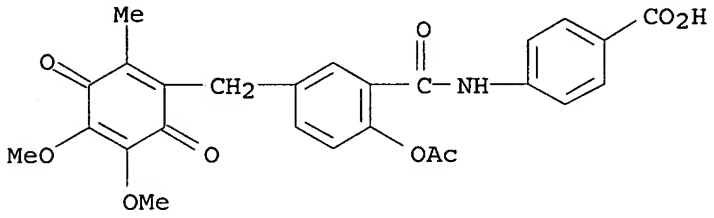
RN 464215-34-7 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-(2,4-dichlorophenyl)-3-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



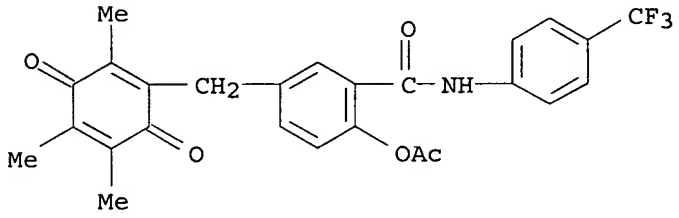
RN 464215-46-1 HCAPLUS
CN Benzoic acid, 4-[[2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]benzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 464215-47-2 HCAPLUS
CN Benzoic acid, 4-[[2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]benzoyl]amino]- (9CI) (CA INDEX NAME)



RN 464215-92-7 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-[4-(trifluoromethyl)phenyl]-5-[(2,4,5-trimethyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



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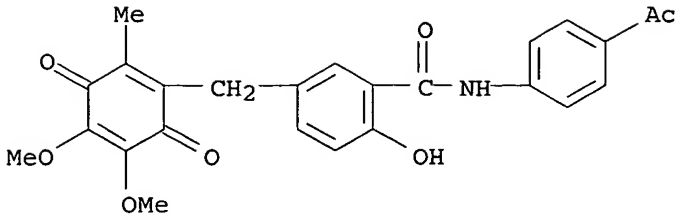
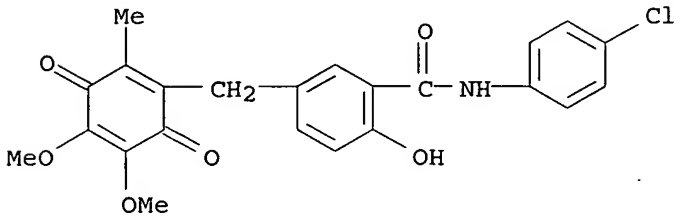
464215-49-4P 464215-72-3P 464215-93-8P
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid derivs. as nuclear factor κB inhibitors)
RN 464214-68-4 HCAPLUS
CN Benzamide, N-(4-acetylphenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



RN 464214-69-5 HCAPLUS
CN Benzamide, N-(4-chlorophenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



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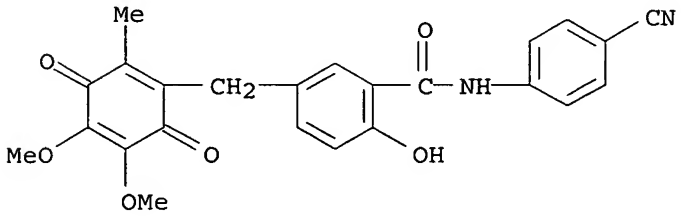
CN Benzamide, N-(4-cyanophenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



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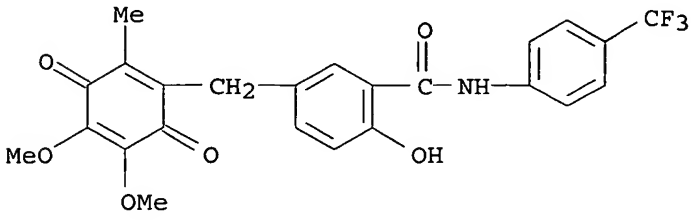
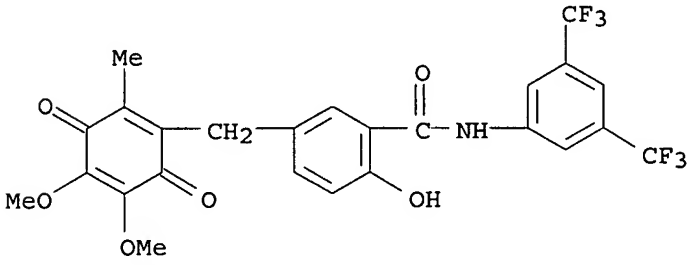
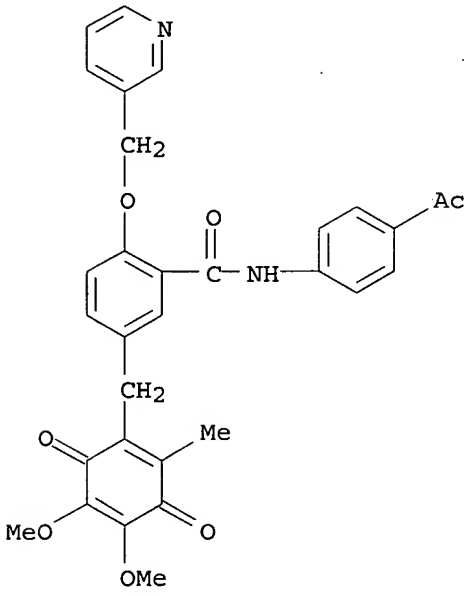


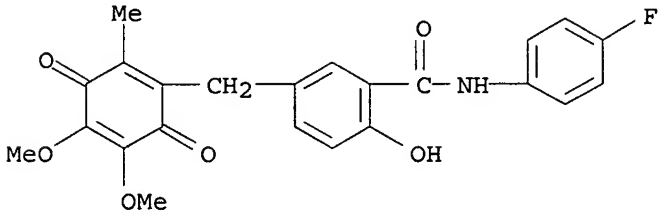
RN 464214-75-3 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



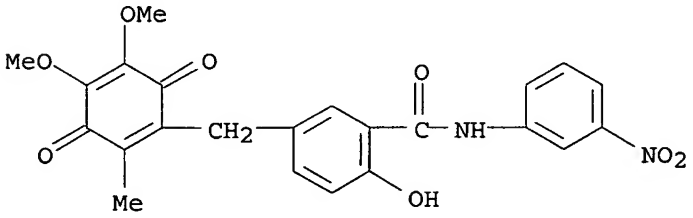
RN 464214-87-7 HCAPLUS
CN Benzamide, N-(4-acetylphenyl)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-(3-pyridinylmethoxy)- (9CI) (CA INDEX NAME)



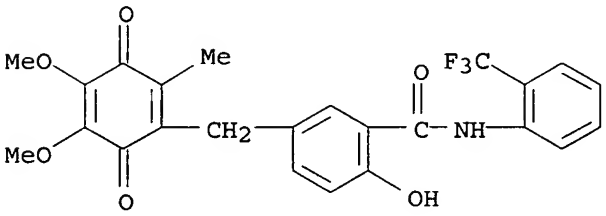
RN 464215-00-7 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-(4-fluorophenyl)-2-hydroxy- (9CI) (CA INDEX NAME)



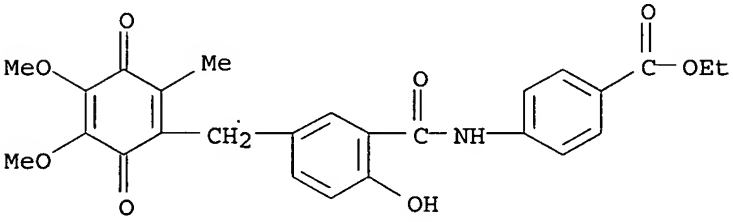
RN 464215-02-9 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-(3-nitrophenyl)- (9CI) (CA INDEX NAME)



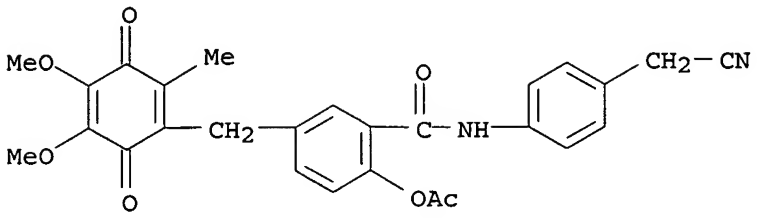
RN 464215-04-1 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



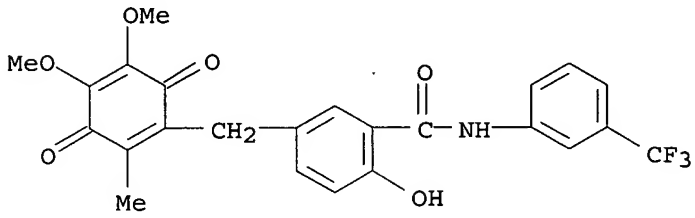
RN 464215-06-3 HCAPLUS
CN Benzoic acid, 4-[[5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxybenzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



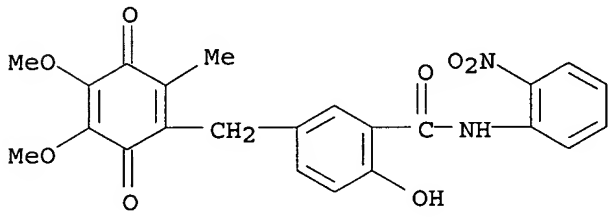
RN 464215-07-4 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-[4-(cyanomethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



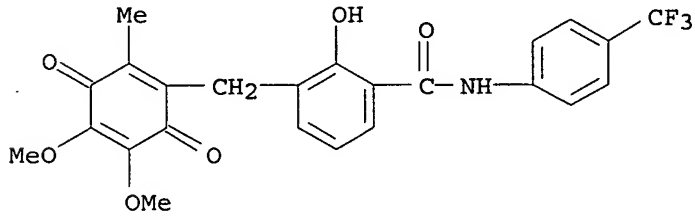
RN 464215-10-9 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



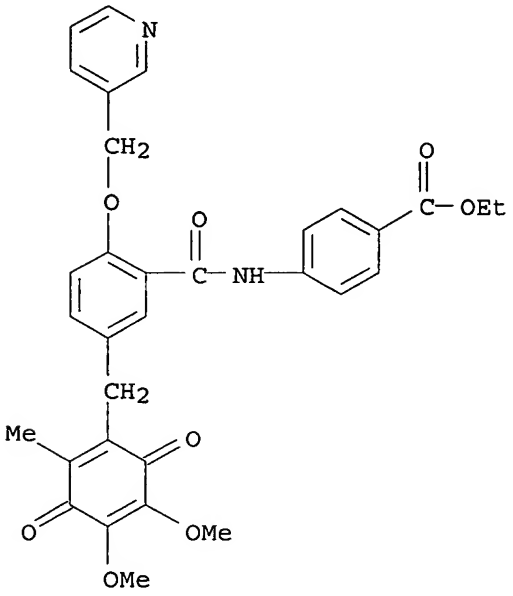
RN 464215-12-1 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-(2-nitrophenyl)- (9CI) (CA INDEX NAME)



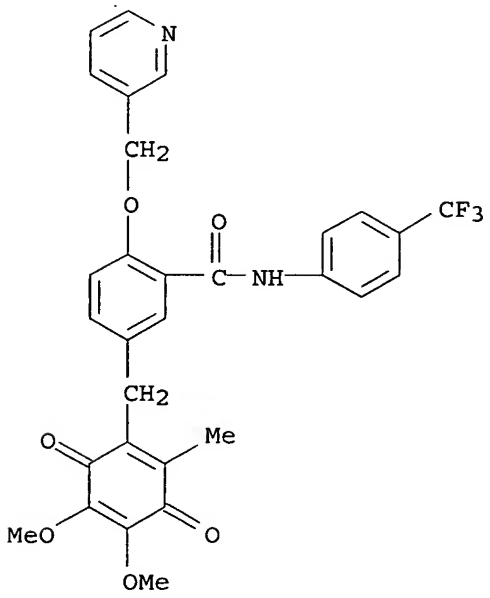
RN 464215-24-5 HCAPLUS
CN Benzamide, 3-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



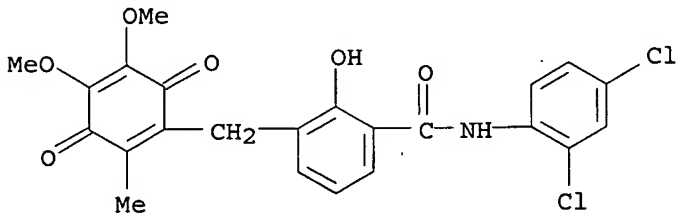
RN 464215-25-6 HCAPLUS
CN Benzoic acid, 4-[[5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-(3-pyridinylmethoxy)benzoyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



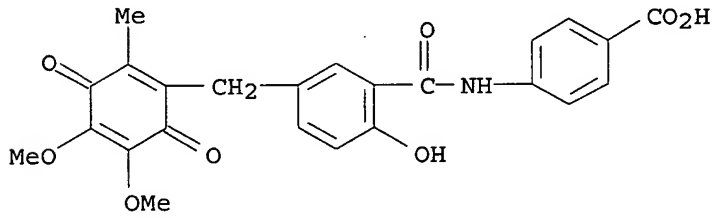
RN 464215-30-3 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-(3-pyridinylmethoxy)-N-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



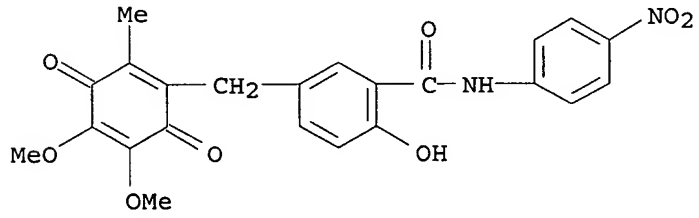
RN 464215-35-8 HCAPLUS
CN Benzamide, N-(2,4-dichlorophenyl)-3-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (9CI) (CA INDEX NAME)



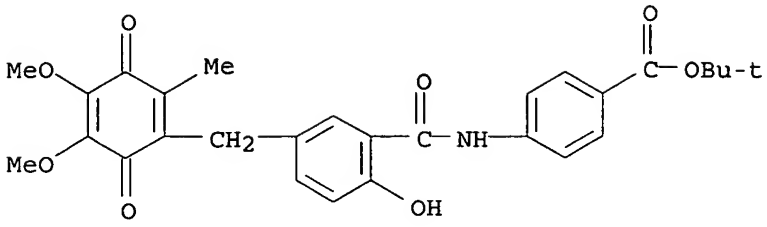
RN 464215-48-3 HCAPLUS
CN Benzoic acid, 4-[[5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxybenzoyl]amino]- (9CI) (CA INDEX NAME)



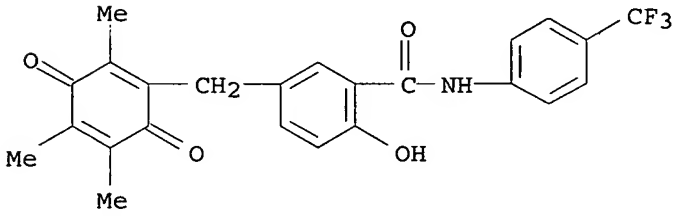
RN 464215-49-4 HCAPLUS
CN Benzamide, 5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 464215-72-3 HCAPLUS
CN Benzoic acid, 4-[[5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxybenzoyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 464215-93-8 HCAPLUS
CN Benzamide, 2-hydroxy-N-[4-(trifluoromethyl)phenyl]-5-[(2,4,5-trimethyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 8 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:487387 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 137:63257
TITLE: Preparation of benzamides as inhibitors of production and release of inflammatory cytokines
INVENTOR(S): Muto, Susumu; Nagano, Tatsuo; Saotome, Tomomi; Itai, Akiko
PATENT ASSIGNEE(S): Institute of Medicinal Molecular Design Inc., Japan
SOURCE: PCT Int. Appl., 313 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002049632	A1	20020627	WO 2001-JP11084	20011218 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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EP 1352650 A1 20031015 EP 2001-271124 20011218 <--
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PRIORITY APPLN. INFO.: JP 2000-383202 A 20001218 <--
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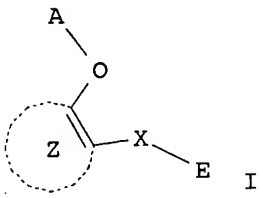
OTHER SOURCE(S): MARPAT 137:63257
GI



I

AB The title compds. I (wherein X is a connecting group; A is hydrogen or acetyl; E is aryl or heteroaryl; and Z is arene or heteroarene) are prepared In an in vitro test using cells, 5-chloro-2-hydroxy-N-(4-methoxynaphthalen-2-yl)benzamide at 1 μg/mL gave 95.1% inhibition of NF-κB activation.

IC ICM A61K031-055
ICS A61K031-166; A61K031-12; A61K031-18; A61K031-167; A61K031-136; A61K031-17; A61K031-695; A61K031-5375; A61K031-357; A61K031-404; A61K031-44; A61K031-498; A61K031-403; A61K031-415; A61K031-421; A61K031-422; A61K031-433; A61K031-428; A61K031-505

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25

IT ***Human immunodeficiency virus***
(***HIV*** gene transcription products; preparation of benzamides as inhibitors of gene expression)

IT Interleukin 1
Interleukin 2
Interleukin 6
Interleukin 8
Tumor necrosis factors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of benzamides as inhibitors of gene expression)

IT ***744-58-1P*** 797-15-9P 900-36-7P 906-38-7P 978-62-1P
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RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzamides as inhibitors of production and release of inflammatory cytokines)

IT ***744-58-1P 66816-49-7P 78154-58-2P***
439144-18-0P 439144-19-1P 439144-20-4P
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RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzamides as inhibitors of production and release of inflammatory cytokines)

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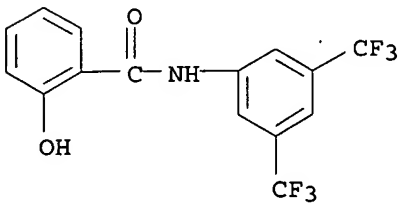

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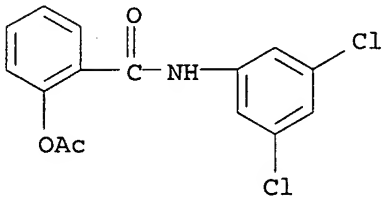

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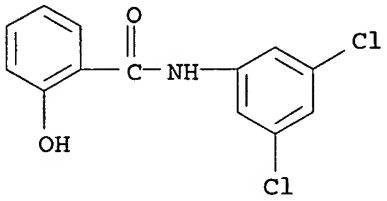

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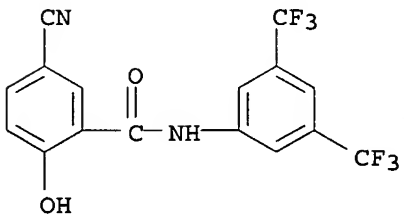

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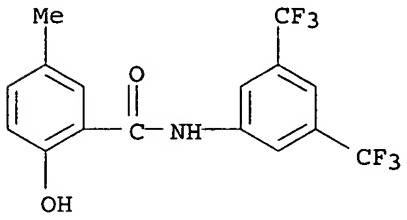

RN 439144-20-4 HCAPLUS
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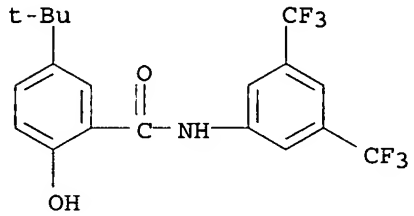

RN 439144-21-5 HCAPLUS
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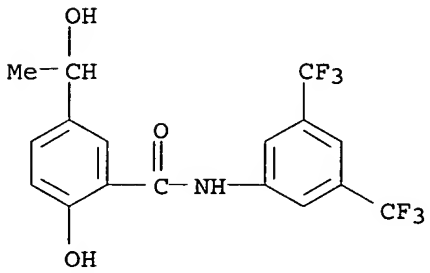
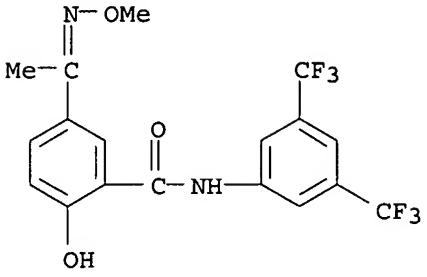
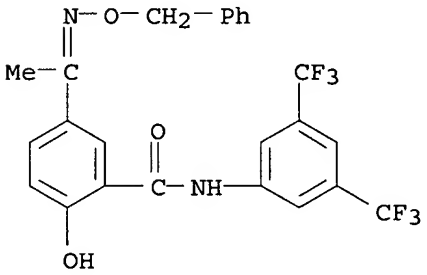


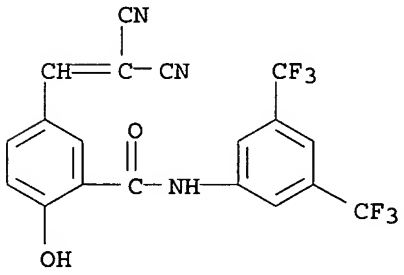
RN 439144-22-6 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-[1-(methoxyimino)ethyl]- (9CI) (CA INDEX NAME)



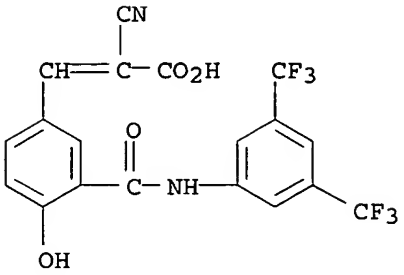
RN 439144-23-7 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-[1-[(phenylmethoxy)imino]ethyl]- (9CI) (CA INDEX NAME)



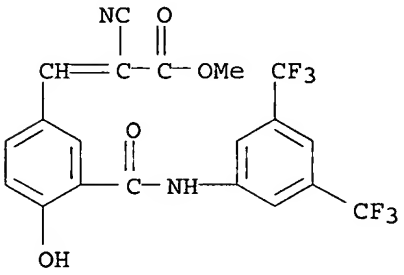
RN 439144-24-8 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-5-(2,2-dicyanoethenyl)-2-hydroxy- (9CI) (CA INDEX NAME)



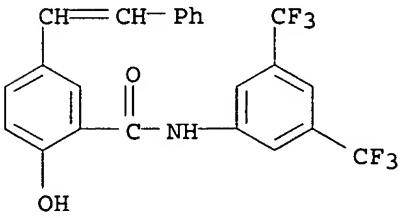
RN 439144-25-9 HCAPLUS
CN 2-Propenoic acid, 3-[3-[[[3,5-bis(trifluoromethyl)phenyl]amino]carbonyl]-4-hydroxyphenyl]-2-cyano- (9CI) (CA INDEX NAME)



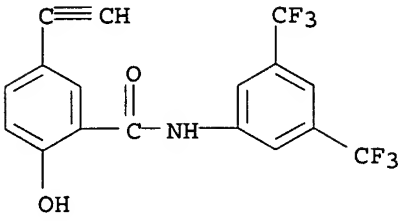
RN 439144-26-0 HCAPLUS
CN 2-Propenoic acid, 3-[3-[[[3,5-bis(trifluoromethyl)phenyl]amino]carbonyl]-4-hydroxyphenyl]-2-cyano-, methyl ester (9CI) (CA INDEX NAME)



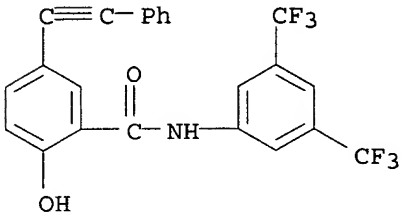
RN 439144-27-1 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(2-phenylethenyl)- (9CI) (CA INDEX NAME)



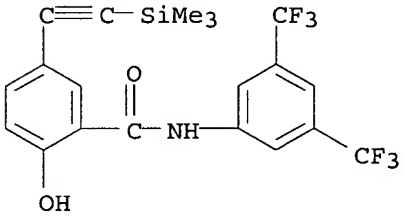
RN 439144-28-2 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-5-ethynyl-2-hydroxy- (9CI) (CA INDEX NAME)



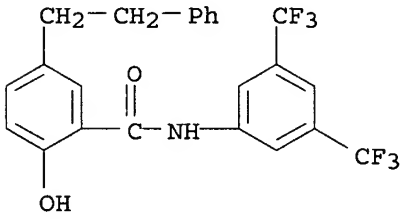
RN 439144-29-3 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(phenylethynyl)-(9CI) (CA INDEX NAME)



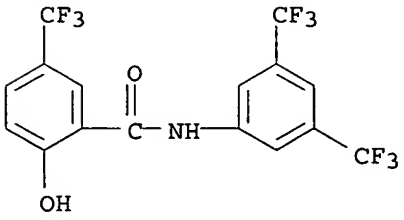
RN 439144-30-6 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-[(trimethylsilyl)ethynyl]- (9CI) (CA INDEX NAME)



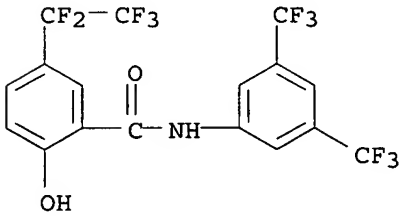
RN 439144-32-8 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(2-phenylethyl)-(9CI) (CA INDEX NAME)



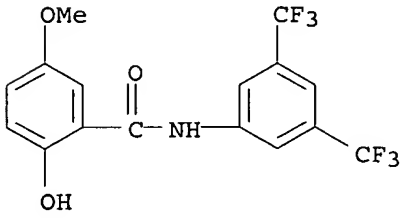
RN 439144-33-9 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



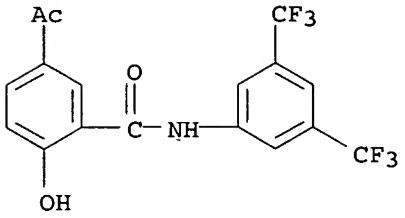
RN 439144-34-0 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(pentafluoroethyl)- (9CI) (CA INDEX NAME)



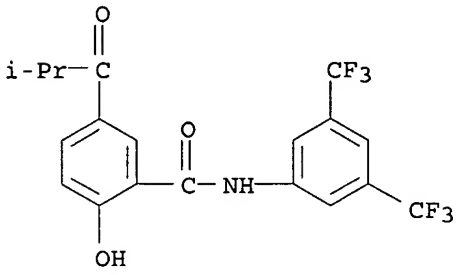
RN 439144-42-0 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-methoxy- (9CI) (CA INDEX NAME)



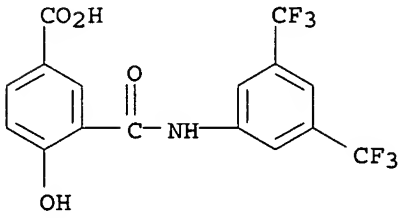
RN 439144-43-1 HCAPLUS
CN Benzamide, 5-acetyl-N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy- (9CI) (CA INDEX NAME)



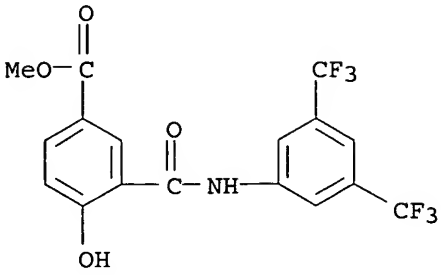
RN 439144-44-2 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(2-methyl-1-oxopropyl)- (9CI) (CA INDEX NAME)



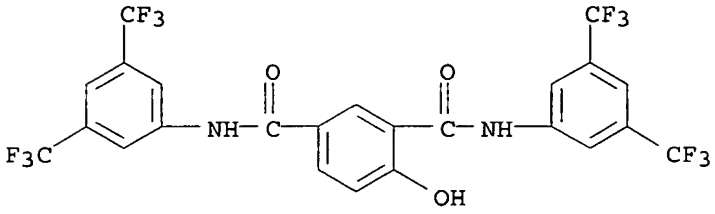
RN 439144-45-3 HCAPLUS
CN Benzoic acid, 3-[[[3,5-bis(trifluoromethyl)phenyl]amino]carbonyl]-4-hydroxy- (9CI) (CA INDEX NAME)



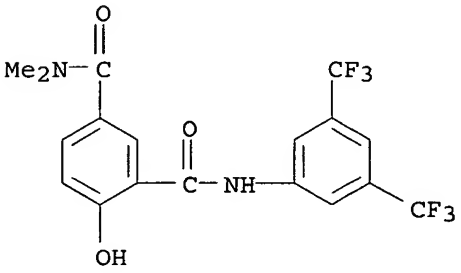
RN 439144-46-4 HCAPLUS
CN Benzoic acid, 3-[[[3,5-bis(trifluoromethyl)phenyl]amino]carbonyl]-4-hydroxy-, methyl ester (9CI) (CA INDEX NAME)



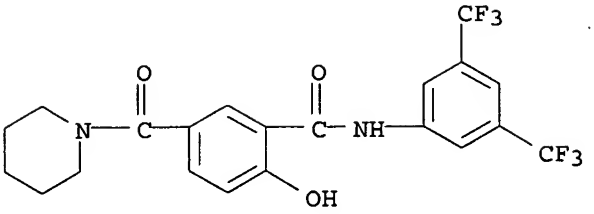
RN 439144-47-5 HCAPLUS
CN 1,3-Benzenedicarboxamide, N,N'-bis[3,5-bis(trifluoromethyl)phenyl]-4-hydroxy- (9CI) (CA INDEX NAME)



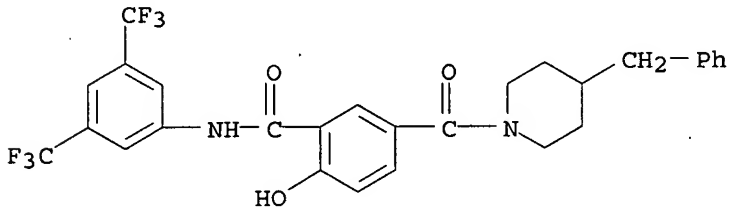
RN 439144-48-6 HCAPLUS
CN 1,3-Benzenedicarboxamide, N3-[3,5-bis(trifluoromethyl)phenyl]-4-hydroxy-N1,N1-dimethyl- (9CI) (CA INDEX NAME)



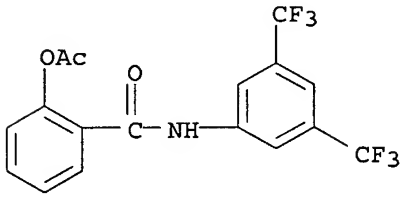
RN 439144-49-7 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-(1-piperidinylcarbonyl)- (9CI) (CA INDEX NAME)



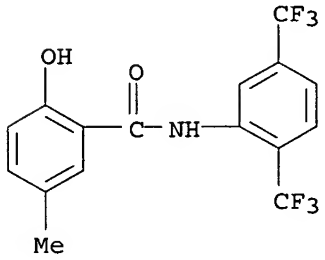
RN 439144-50-0 HCAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-[[4-(phenylmethyl)-1-piperidinyl]carbonyl]- (9CI) (CA INDEX NAME)



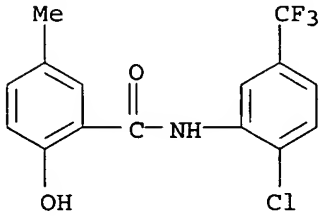
RN 439144-60-2 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-[3,5-bis(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



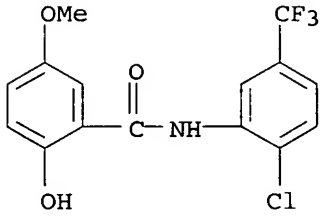
RN 439144-67-9 HCAPLUS
CN Benzamide, N-[2,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-methyl- (9CI) (CA INDEX NAME)



RN 439144-95-3 HCAPLUS
CN Benzamide, N-[2-chloro-5-(trifluoromethyl)phenyl]-2-hydroxy-5-methyl-
(9CI) (CA INDEX NAME)



RN 439144-96-4 HCAPLUS
CN Benzamide, N-[2-chloro-5-(trifluoromethyl)phenyl]-2-hydroxy-5-methoxy-
(9CI) (CA INDEX NAME)



RN 439144-97-5 HCAPLUS
CN Benzamide, N-[4-chloro-3-(trifluoromethyl)phenyl]-2-hydroxy-5-methyl-
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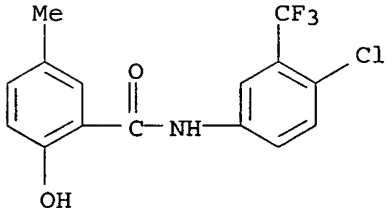

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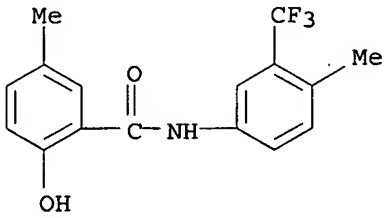

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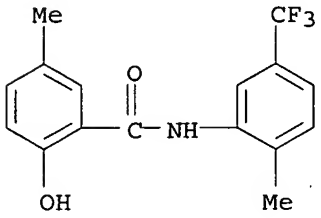
CN Benzamide, 2-hydroxy-5-methyl-N-[2-methyl-5-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 439145-08-1 HCAPLUS
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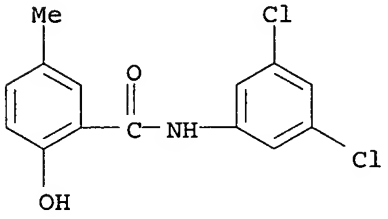

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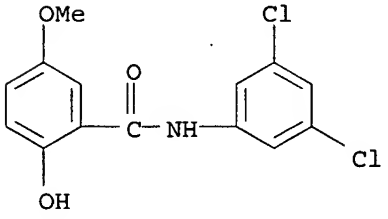

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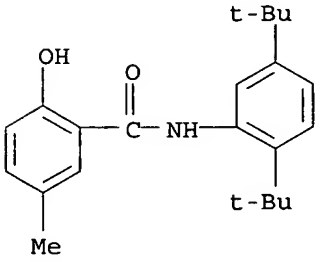

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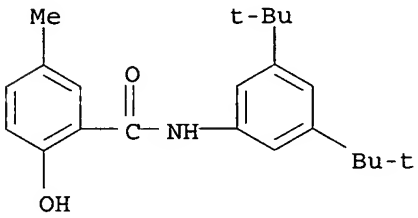

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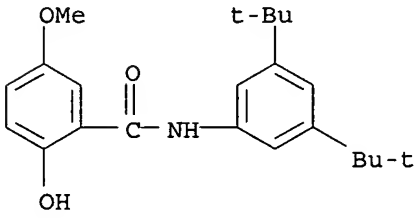

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 9 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2002:31445 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 136:86057
TITLE: Preparation of aza-bridged-bicyclic amino acid derivatives as α4 integrin antagonists
INVENTOR(S): Dyatkin, Alexey B.; Maryanoff, Bruce E.; Hoekstra, William J.; He, Wei; Kinney, William A.

PATENT ASSIGNEE(S): Ortho McNeil Pharmaceutical, Inc., USA
SOURCE: PCT Int. Appl., 99 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 2002002556	A2	20020110	WO 2001-US20857		20010629	<--
WO 2002002556	A3	20020718				
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
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EP 1303492	A2	20030423	EP 2001-952331		20010629	<--
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ZA 2003000794	A	20040429	ZA 2003-794		20030129	<--
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OTHER SOURCE(S): MARPAT 136:86057
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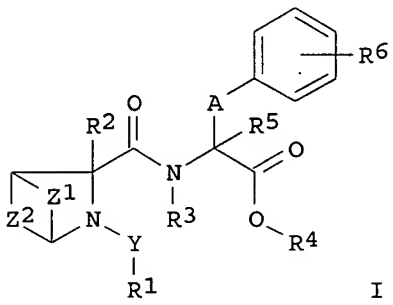

I

AB Aza-bridged-bicyclic amino acid derivs. I [Y = a bond, CO, CO2, CONH, SO2; R1 = (un)substituted cycloalkyl, heterocyclyl, aryl, haloalkyl, alkyl, alkenyl, alkynyl, heteroaryl; R2, R3, R4 and R5 = H, (un)substituted alkyl, a bond when forming a monocyclic ring; R6 = one to three substituents selected from halogen, alkoxy, (un)substituted cycloalkyl,

heterocyclyl, aryl, haloalkyl heteroaryl, amino, arylsulfonyl, etc.; A = (un)substituted alkylene; Z1 and Z2 = (un)substituted alkylene or alkenylene] were prepared as α4β1 and α4β7 integrin receptor antagonists. Thus, condensation of benzenesulfonyl isocyanate with Et glyoxalate, followed by cycloaddn. with cyclohexadiene, hydrogenation, saponification, coupling with (S)-4-nitrophenylalanine Me ester, reduction of the nitro group, acylation with 2,6-dichlorobenzoyl chloride and ester saponification gave 4-[(2,6-dichlorobenzoyl)amino]-N-[[(3S)-2-(phenylsulfonyl)-2-azabicyclo[2.2.2]oct-3-yl]carbonyl]-L-phenylalanine, which showed IC50 = 21nM in Ramos cell adhesion assay.

IC ICM C07D451-00

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 27, 63

IT Anti-inflammatory agents
Antiasthmatics
Autoimmune disease
Cytotoxic agents
Psoriasis
Rheumatoid arthritis
Transplant rejection
(preparation of aza-bridged-bicyclic amino acid derivs. as α4 integrin antagonists)

IT 387336-52-9P 387336-59-6P 387336-60-9P 387336-61-0P 387336-62-1P
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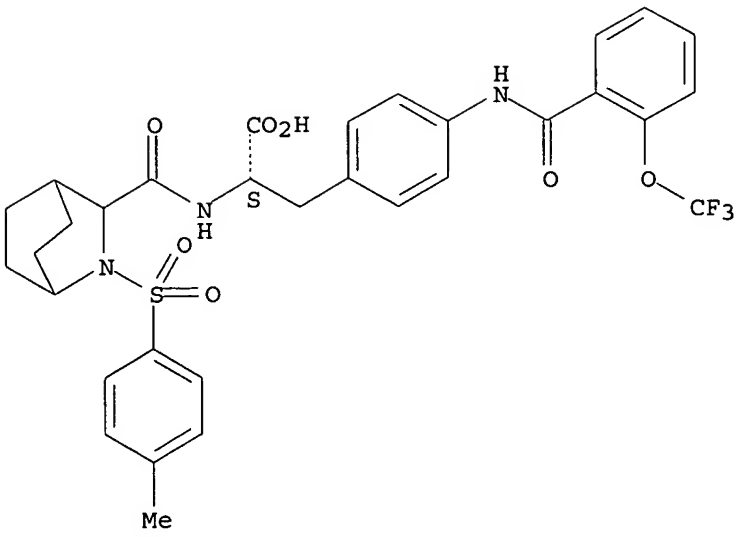
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aza-bridged-bicyclic amino acid derivs. as α4 integrin antagonists)

IT ***387336-67-6P***
RL: ***PAC (Pharmacological activity)***; SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aza-bridged-bicyclic amino acid derivs. as α4 integrin antagonists)

RN 387336-67-6 HCAPLUS

CN L-Phenylalanine, N-[[2-[(4-methylphenyl)sulfonyl]-2-azabicyclo[2.2.2]oct-3-yl]carbonyl]-4-[[2-(trifluoromethoxy)benzoyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L101 ANSWER 10 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:795092 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:331263
TITLE: Preparation of benzoic acid amides as inhibitors of tyrosine kinase KDR and FLT.
INVENTOR(S): Huth, Andreas; Seidelmann, Dieter; Thierauch, Karl-Heinz
PATENT ASSIGNEE(S): Schering A.-G., Germany
SOURCE: Ger. Offen., 26 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10021246	A1	20011031	DE 2000-10021246	20000425 <--
CA 2406392	AA	20011101	CA 2001-2406392	20010424 <--
WO 2001081311	A1	20011101	WO 2001-EP4627	20010424 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1280776	A1	20030205	EP 2001-925566	20010424 <--
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BR 2001010246	A	20030305	BR 2001-10246	20010424 <--
EE 200200609	A	20040415	EE 2002-609	20010424 <--
JP 2004512259	T2	20040422	JP 2001-578406	20010424 <--
NZ 521681	A	20060331	NZ 2001-521681	20010424 <--

BG 107212	A	20030530	BG 2002-107212		20021023 <--
NO 2002005102	A	20021217	NO 2002-5102		20021024 <--
ZA 2002009494	A	20040714	ZA 2002-9494		20021121 <--
PRIORITY APPLN. INFO.:			DE 2000-10021246	A	20000425 <--
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OTHER SOURCE(S): MARPAT 135:331263

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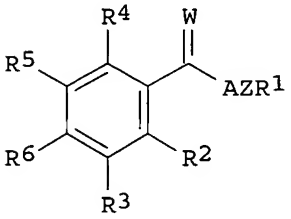

I

AB Title compds. [I; A = NR7; W = O, S, H2, NR8; Z = bond, NR10, N, alkyl, etc.; R1 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl, heteroaryl; R2, R3 = H, OH, XR11; X = alkyl, alkenyl, alkynyl; R11 = (substituted) aryl, heteroaryl; R4-R6 = H, halo, (substituted) alkoxy, alkyl, cycloalkyl; R4R5 = OCH2O; R7, R8, R10 = H, alkyl], were prepared Thus, Me 2-(4-pyridylethyl)benzoate (preparation given) and 4-chloroaniline in PhMe at 4° were treated with Me3Al in hexane followed by warming to 120° to give N-(4-chlorophenyl) 2-(4-pyridylethyl)benzamide. I inhibited VEGFRI (FLT) kinase and VEGFRII (KDR) kinase with IC50 = 0.05-2 μM and 0.2-5 μM, resp.

IC ICM A61K031-44
ICS A61K031-47; A61K031-16

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27

ST benzoic acid amide prepn tyrosine kinase KDR FLT inhibitor; glaucoma treatment benzoic acid amide; diabetic retinopathy treatment benzoic acid amide; ***anticancer*** drug benzoic acid amide; psoriasis treatment benzoic acid amide; antiarthritic benzoic acid amide; pyridylethylbenzamide prepn tyrosine kinase KDR FLT prepn

IT ***Blood vessel, neoplasm***
(angiofibroma, treatment; preparation of benzoic acid amides as inhibitors of tyrosine kinase KDR and FLT)

IT ***Blood vessel, neoplasm***
(hemangioma, treatment; preparation of benzoic acid amides as inhibitors of tyrosine kinase KDR and FLT)

IT 369388-40-9P 369388-42-1P 369388-45-4P 369388-47-6P 369388-49-8P
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369389-39-9P

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid amides as inhibitors of tyrosine kinase KDR and FLT)

IT ***369389-20-8P 369389-22-0P 369389-24-2P 369389-26-4P 369389-28-6P 369389-35-5P 369389-36-6P 369389-37-7P 369389-38-8P 369389-39-9P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid amides as inhibitors of tyrosine kinase KDR and FLT)

RN 369389-20-8 HCAPLUS
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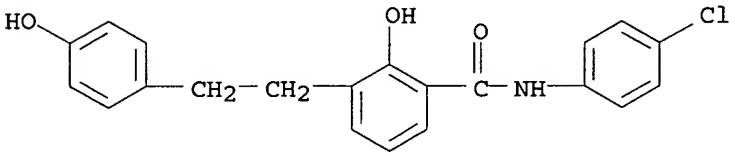

RN 369389-22-0 HCAPLUS
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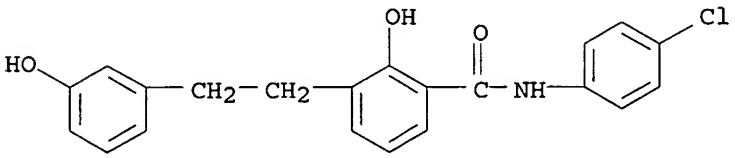

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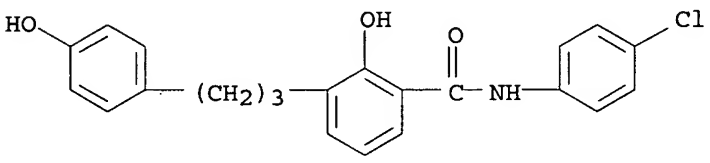

RN 369389-26-4 HCAPLUS

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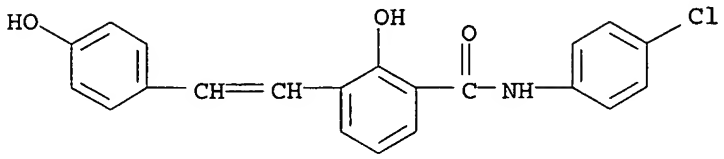
(9CI) (CA INDEX NAME)



RN 369389-28-6 HCAPLUS
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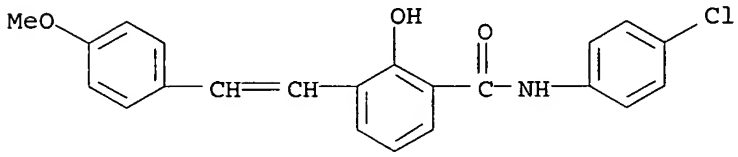
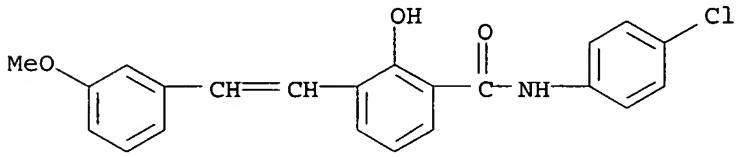
(9CI) (CA INDEX NAME)



RN 369389-35-5 HCAPLUS
CN Benzamide, N-(4-chlorophenyl)-2-hydroxy-3-[2-(3-methoxyphenyl)ethenyl]-
(9CI) (CA INDEX NAME)



RN 369389-36-6 HCAPLUS
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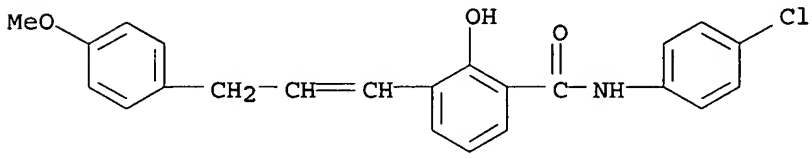
(9CI) (CA INDEX NAME)



RN 369389-37-7 HCAPLUS
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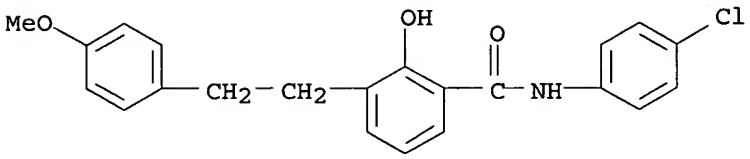
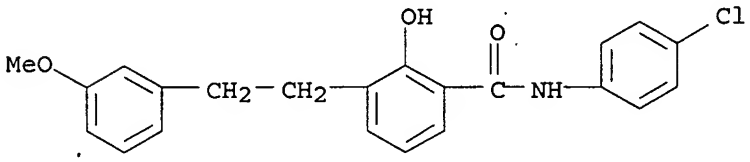
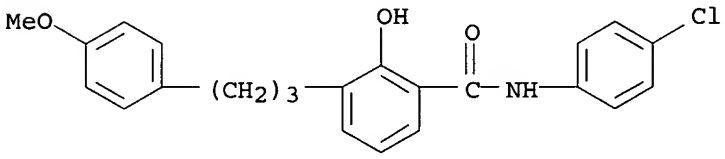
(9CI) (CA INDEX NAME)



RN 369389-38-8 HCAPLUS
CN Benzamide, N-(4-chlorophenyl)-2-hydroxy-3-[2-(3-methoxyphenyl)ethyl]-(9CI) (CA INDEX NAME)



RN 369389-39-9 HCAPLUS
CN Benzamide, N-(4-chlorophenyl)-2-hydroxy-3-[3-(4-methoxyphenyl)propyl]-(9CI) (CA INDEX NAME)



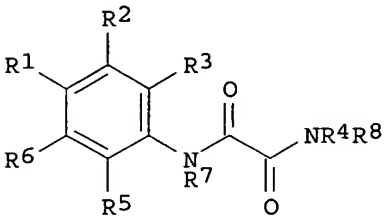
L101 ANSWER 11 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:631913 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:195556
TITLE: Preparation of azolylphenyl oxamides as inosine monophosphate dehydrogenase (IMPDH) inhibitors
INVENTOR(S): Broadhurst, Michael John; Hill, Christopher Huw; Hurst, David Nigel; Jones, Philip Stephen; Kay, Paul Brittain; Kilford, Ian Reginald; Mckinnell, Robert Murray
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.
SOURCE: Eur. Pat. Appl., 256 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1127883	A2	20010829	EP 2001-103521	20010216 <--

EP 1127883	A3	20020807				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO						
US 2002052513	A1	20020502	US 2001-779116		20010208	<--
US 6867299	B2	20050315				
CA 2337588	AA	20010824	CA 2001-2337588		20010220	<--
HR 2001000127	A1	20011231	HR 2001-127		20010221	<--
NO 2001000900	A	20010827	NO 2001-900		20010222	<--
CN 1310179	A	20010829	CN 2001-104906		20010223	<--
BR 2001000790	A	20010925	BR 2001-790		20010223	<--
JP 2001261663	A2	20010926	JP 2001-51064		20010226	<--
PRIORITY APPLN. INFO.:			GB 2000-4392	A	20000224	<--
			GB 2000-15877	A	20000628	<--
			GB 2000-20322	A	20000817	<--

OTHER SOURCE(S): MARPAT 135:195556

GI



I

AB Title compds. (I; R1 = heterocyclyl; R2 = H, alkyl, alkoxy, halo, OH, cyano; R3 = H, alkyl, alkoxy, halo, cyano; R4 = H, alkyl, cycloalkyl, aryl, heterocyclyl; R5 = H, alkyl, alkoxy, halo, cyano; R6 = H, alkyl, alkoxy, halo, cyano; R7, R8 = H, alkyl; R4R8N = heterocyclyl), were prepared Thus, 1,1-dimethyl-3-(4-nitrophenoxy)propylamine (preparation given) was coupled with N-[3-methoxy-4-(5-oxazolyl)phenyl]oxamic acid in the presence of 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide and 1-hydroxy-7-azabenzotriazole to give N-[3-methoxy-4-(5-oxazolyl)phenyl]-N'-[1,1-dimethyl-3-(4-nitrophenoxy)propyl]oxalamide. Tested I inhibited IMPDH with IC50 = 0.010-0.277 μM. I can be used for treating immune mediated conditions or diseases, viral diseases, bacterial diseases, parasitic diseases, inflammation, inflammatory diseases, hyperproliferative vascular diseases, ***tumors***, and ***cancer***.

IC ICM C07D263-32
ICS C07D413-12; C07D417-12; A61K031-421; A61K031-422; A61K031-4439; A61K031-454; A61P029-00; A61P031-00; A61P035-00; A61P037-00

CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST azolylphenyl oxamide prepn inosine monophosphate dehydrogenase inhibitor; IMPDH inhibitor azolylphenyl oxamide prepn; immune mediated disease treatment azolylphenyl oxamide; hyperproliferative vascular disease treatment azolylphenyl oxamide; ***cancer*** treatment azolylphenyl oxamide; inflammation treatment azolylphenyl oxamide; parasitic disease treatment azolylphenyl oxamide; bacterial disease treatment azolylphenyl oxamide; viral disease treatment azolylphenyl oxamide

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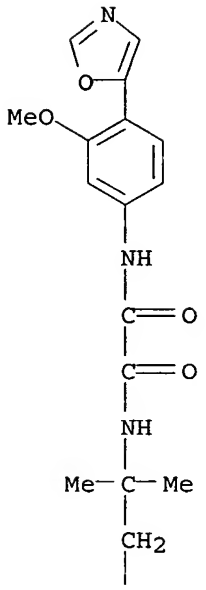
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolylphenyl oxamides as inosine monophosphate dehydrogenase (IMPDH) inhibitors)

IT ***357180-27-9P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azolylphenyl oxamides as inosine monophosphate dehydrogenase (IMPDH) inhibitors)

RN 357180-27-9 HCAPLUS
CN Ethanediamide, N-[2-[4-[(2-methoxybenzoyl)amino]phenyl]-1,1-dimethylethyl]-N'-[3-methoxy-4-(5-oxazolyl)phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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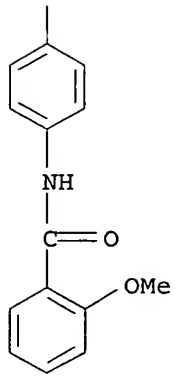

L101 ANSWER 12 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:565016 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:137529
TITLE: Preparation of azepine derivatives as VLA-4 antagonists
INVENTOR(S): Ikegami, Satoru; Inoguchi, Kiyoshi; Fukui, Hideto; Sumita, Yuji; Maruyama, Tatsuya; Watanuki, Mitsuru

PATENT ASSIGNEE(S): Kaken Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055121	A1	20010802	WO 2001-JP521	20010126 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 2000-20358 A 20000128 <--
OTHER SOURCE(S): MARPAT 135:137529
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R1 = H, alkyl, aryl; R2 = H, (CH3)3COCO; R3 = alkylene, divalent aromatic hydrocarbon derivs.; R4 = H, alkyl; X = aromatic hydrocarbon; heterocycle; m = 1, 2, 3; Y = N, O; Z = R8R7R6A1; A1 = CH2, SO2; R6 = alkylene, divalent arylalkane derivs.; R7 = CH2, CO; R8 = alkyl, arylalkyl] and salts are prepared Title compds. or salts of title compds. are used as the active ingredient in remedies having peroral absorbability and exhibiting VLA-4 antagonism. Thus, the title compound II was prepared and biol. tested for VLA-4 antagonism.

IC C07D243-24; C07D267-14; C07D413-12; C07D401-12; C07D403-12; C07D417-12; C07D491-052; C07D471-04; A61K031-553; A61K031-5513; A61P043-00; A61P029-00; A61P019-02; A61P013-12; A61P001-04; A61P037-06; A61P025-00; A61P011-06; A61P037-08; A61P009-10

CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT Anti-inflammatory agents
Antiasthmatics
Antirheumatic agents
(azepines)

IT ***Neoplasm***
(diabetic complication; preparation and use of azepine derivs. as VLA-4 antagonists)

IT Arteriosclerosis
Asthma
Lupus erythematosus
Multiple sclerosis
Rheumatoid arthritis
Transplant and Transplantation
(preparation and use of azepine derivs. as VLA-4 antagonists)

IT 351903-56-5P 351903-57-6P 351903-58-7P 351903-59-8P 351903-60-1P
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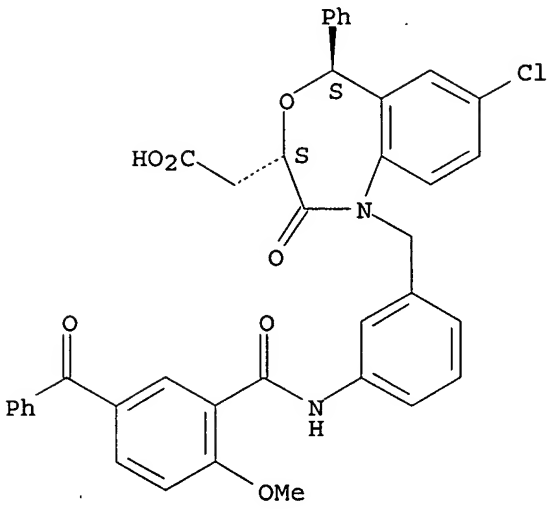
RL: SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azepine derivs. as VLA-4 antagonists)

IT ***352234-86-7P 352234-88-9P***
RL: SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azepine derivs. as VLA-4 antagonists)

RN 352234-86-7 HCAPLUS

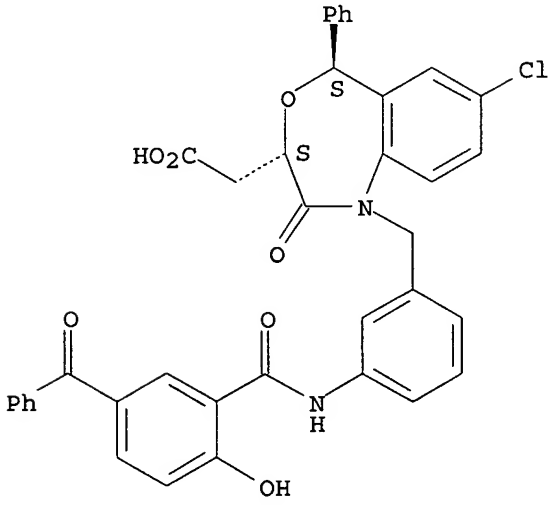
CN 4,1-Benzoxazepine-3-acetic acid, 1-[[3-[(5-benzoyl-2-methoxybenzoyl)amino]phenyl]methyl]-7-chloro-1,2,3,5-tetrahydro-2-oxo-5-phenyl-, (3R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 352234-88-9 HCAPLUS
CN 4,1-Benzoxazepine-3-acetic acid, 1-[[3-[(5-benzoyl-2-hydroxybenzoyl)amino]phenyl]methyl]-7-chloro-1,2,3,5-tetrahydro-2-oxo-5-phenyl-, (3R,5R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 13 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:545674 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:137516
TITLE: Synthesis of heteroarylbenzamides and analogs used for inhibiting protein kinases
INVENTOR(S): Bender, Steven Lee; Bhumralkar, Dilip; Collins, Michael Raymond; Cripps, Stephan James; Deal, Judith

Gail; Nambu, Mitchell David; Palmer, Cynthia Louise; Peng, Zhengwei; Varney, Michael David; Jia, Lei
PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 237 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001053274	A1	20010726	WO 2001-US1723		20010119 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2394703	AA	20010726	CA 2001-2394703		20010119 <--
US 2002103203	A1	20020801	US 2001-764306		20010119 <--
US 6635641	B2	20031021			
EP 1252146	A1	20021030	EP 2001-906592		20010119 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
BR 2001008025	A	20021105	BR 2001-8025		20010119 <--
JP 2003529558	T2	20031007	JP 2001-553276		20010119 <--
US 2004092747	A1	20040513	US 2003-621979		20030717 <--
PRIORITY APPLN. INFO.:			US 2000-177059P	P	20000121 <--
			US 2001-764306	A3	20010119 <--
			WO 2001-US1723	W	20010119 <--

OTHER SOURCE(S): MARPAT 135:137516
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [Z = CH, NH; Q = moiety such that ring A is (un)substituted mono- or bicyclic heteroaryl which has at least 2 carbon atoms in the heteroaryl ring system; X = CH2, O, S, NH; Y = CH2, O, S, provided at least one of X and Y = CH2 or X and Y form a cyclopropyl ring; R2-3 = H, Me, halo, CF3, CN; R4 = CONHR5, NHCOR6; where R5 = (un)substituted aryl, heteroaryl, cycloalkyl, etc.; R6 = (un)substituted aryl, heteroaryl, cycloalkyl, etc] are prepared Examples include synthetic procedures for over 150 compds., 11 biol. assays and 3 sample formulations. For instance, 3-mercaptobenzoic acid was treated with α-chloro-N-methoxy-N-methylacetamide followed by carbodiimide coupling to 2-methyl-6-aminoquinoline to give II. II was converted to a β-thiono-ketone with thioacetanilide/n-BuLi followed by treatment with hydrazine to give pyrazole III. III gave 85% inhibition of an lck protein tyrosine kinase at 5 μM and had Ki = 2.21 nM for VEGF-R2Δ50. Treatment of ***cancer*** as well as other disease states associated with unwanted angiogenesis and/or cellular proliferation, such as diabetic retinopathy, neovascular glaucoma, rheumatoid arthritis,

and psoriasis are claimed uses of the invention.

IC ICM C07D241-18
ICS A61K031-495; A61P035-00; C07D241-12; C07D249-12; C07D487-04; C07D231-12; C07D471-04; C07D213-30; C07D215-14; C07D217-16; C07D213-75; C07D405-12; C07D401-12; C07D413-12

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 25, 63

IT 351322-40-2P 351322-41-3P 351322-42-4P 351322-43-5P 351322-44-6P
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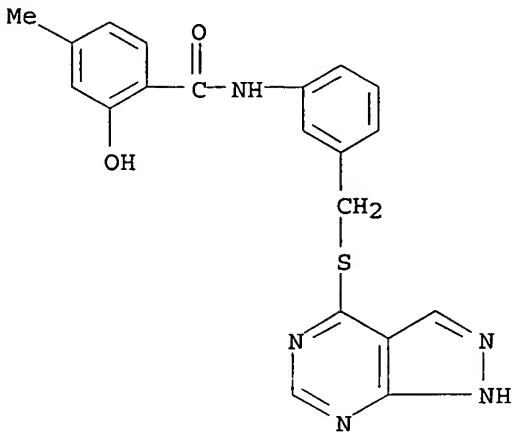
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of heteroarylbenzamides used for inhibiting protein kinases)

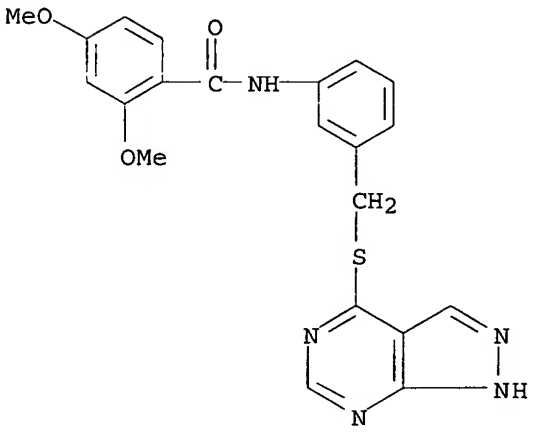
IT ***351323-77-8P 351323-84-7P 351323-87-0P***
351323-90-5P 351324-11-3P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis of heteroarylbenzamides used for inhibiting protein kinases)

RN 351323-77-8 HCAPLUS

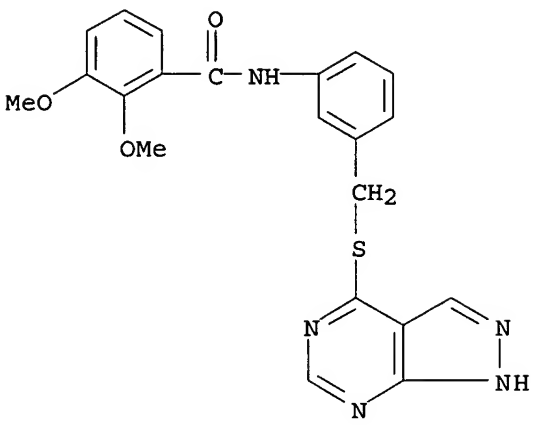
CN Benzamide, 2-hydroxy-4-methyl-N-[3-[(1H-pyrazolo[3,4-d]pyrimidin-4-ylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)



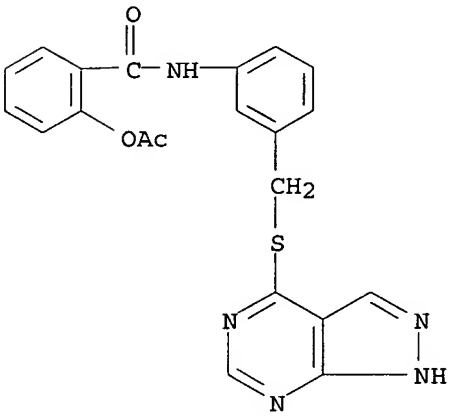
RN 351323-84-7 HCAPLUS
CN Benzamide, 2,4-dimethoxy-N-[3-[(1H-pyrazolo[3,4-d]pyrimidin-4-ylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)



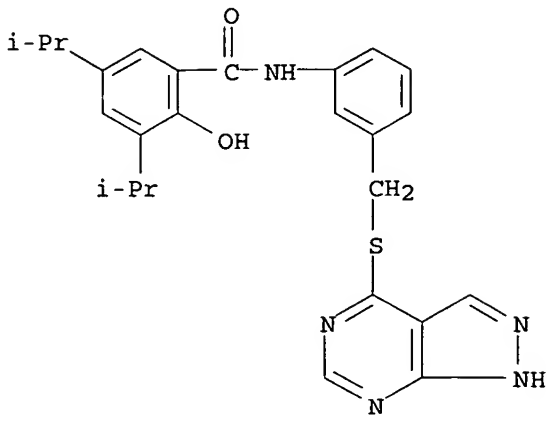
RN 351323-87-0 HCAPLUS
CN Benzamide, 2,3-dimethoxy-N-[3-[(1H-pyrazolo[3,4-d]pyrimidin-4-ylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 351323-90-5 HCAPLUS
CN Benzamide, 2-(acetyloxy)-N-[3-[(1H-pyrazolo[3,4-d]pyrimidin-4-ylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)



RN 351324-11-3 HCAPLUS
CN Benzamide, 2-hydroxy-3,5-bis(1-methylethyl)-N-[3-[(1H-pyrazolo[3,4-d]pyrimidin-4-ylthio)methyl]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 14 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:453001 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:46002
TITLE: Synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors for treatment of ***cancer*** related disorders
INVENTOR(S): Allen, Darin Arthur; McGee, Danny Peter Claude; Spencer, Jeffrey R.
PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 79 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001044172	A1	20010621	WO 2000-US34211	20001214 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2394639	AA	20010621	CA 2000-2394639	20001214 <--
AU 2001021086	A5	20010625	AU 2001-21086	20001214 <--
US 2002052343	A1	20020502	US 2000-737687	20001214 <--
EP 1242366	A1	20020925	EP 2000-984472	20001214 <--
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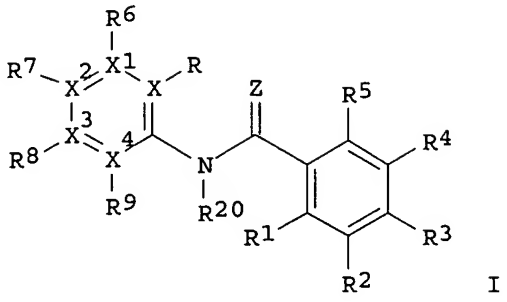
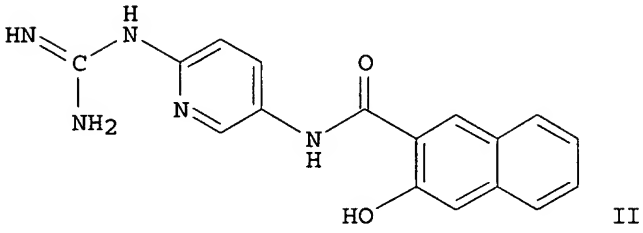
US 2003232789	A1	20031218	US 2002-149864	20021024 <--
PRIORITY APPLN. INFO.:			US 1999-170916P P	19991215 <--
			WO 2000-US34211 W	20001214 <--

OTHER SOURCE(S): MARPAT 135:46002

GI



I



II

AB Compds. I and a process for their synthesis are claimed [wherein; R1 = OH, CO2H, ester, CH2O-, (O)SO3H, sulfonate ester or OP(O)(OH)2 or esters thereof; R2-5 = H, SH, O-, halo, ester, amide, (substituted)aryl, heterocyclyl, etc.; R, R6, R9 = H, halo, CN, (halo)alkyl, NO2, O-aryl/alkyl or R, R6 taken together form (un)saturated (un)substituted C4; R7, R8 = OH, CF3, H, CO2H, NO2, (O)alkyl/aryl, halo, cyano, (substituted)guanidino/amidino, imidazolin-2-yl, N-amidino(morpholine/piperidine), etc.; X includes C; X1-4 = C or N; R20 = H or OH; Z = O, S, CH2, N-, H(CO2H), H(CH2OH), etc.; with the proviso that at least 2 of X1-4 = C and when any of X1-4 = N the corresponding substituent does not exist]. Data for over 40 synthetic examples is provided. The process claimed involves a selective acylation of an amino group and is exemplified by the synthesis of II. 3-Acetoxy-2-chlorocarbonylnaphthalene was prepared from the corresponding carboxylic acid and coupled, in the presence of N,N-dimethylacetamide (or other selected acetamides), to N-(5-aminopyridin-2-yl)guanidine hydrochloride to give the acetoxy derivative of II. The acetoxy derivative was treated with 1M HCl for 2 h to provide II, isolated as the HCl salt. Compds. of the invention are inhibitors of serine proteases, urokinase (uPA), factor Xa (FXa) and/or factor VIIa (FVIIa). Guanidine II had Ki = 0.326 μM for urokinase and Ki = 130 μM for FXa. Compds. I are ***anticancer*** agents and/or anticoagulants and also used for the treatment or prevention of thromboembolic disorders in mammals.

IC ICM C07C257-18
ICS C07C279-18; A61K031-155; A61P007-02; A61P035-00

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63

ST Xa urokinase inhibitor ***anticancer*** anticoagulant guanidine amidine amide prepn

IT ***Neoplasm***

(related disorders; prevention/treatment; synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors)

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RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors)

IT ***345236-73-9***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(drug candidate; synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors)

IT ***345236-68-2P 345236-71-7P 345236-77-3P***
345236-78-4P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors)

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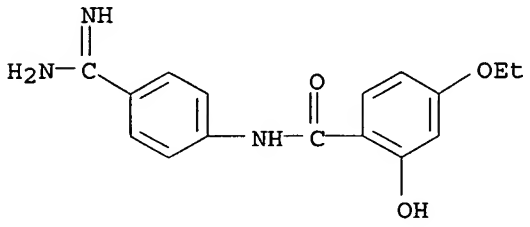

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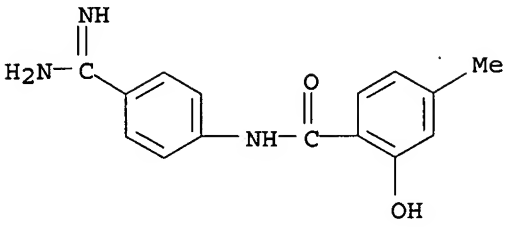

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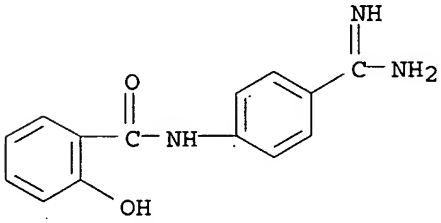

RN 345236-78-4 HCAPLUS
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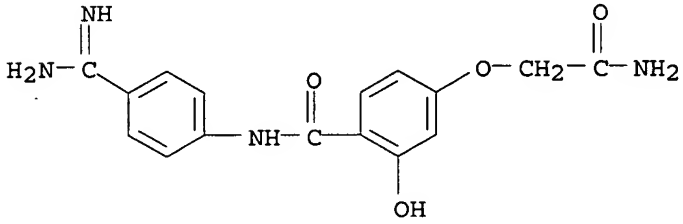
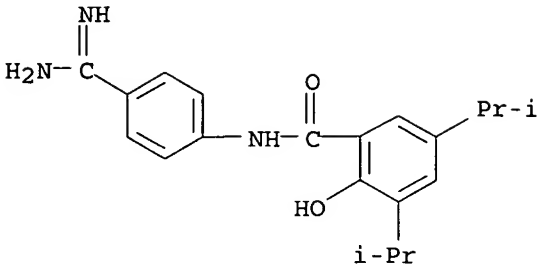


IT ***345236-73-9***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(drug candidate; synthesis and use of amidino/guanidino-arylamino salicylamides as serine protease inhibitors)
RN 345236-73-9 HCAPLUS
CN Benzamide, N-[4-(aminoiminomethyl)phenyl]-2-hydroxy-3,5-bis(1-methylethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 15 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:380546 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 134:367194
TITLE: Preparation of novel phenylalanine derivatives as α4-integrin inhibitors
INVENTOR(S): Tanaka, Yasuhiro; Yoshimura, Toshihiko; Izawa, Hiroyuki; Ejima, Chieko; Kojima, Mitsuhiko; Atake, Yuko; Nakanishi, Eiji; Suzuki, Nobuyasu; Makino, Shingo; Suzuki, Manabu; Murata, Masahiro
PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001036376	A1	20010525	WO 2000-JP8152	20001120 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 2001014165	A5	20010530	AU 2001-14165	20001120 <--
EP 1233013	A1	20020821	EP 2000-976347	20001120 <--
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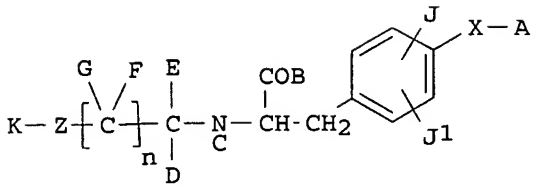
US 2003149083	A1	20030807	US 2002-150067	20020520 <--
US 6855706	B2	20050215		
US 2005070485	A1	20050331	US 2004-986829	20041115 <--

PRIORITY APPLN. INFO.:	JP 1999-328468	A	19991118 <--
	JP 2000-197139	A	20000629 <--
	WO 2000-JP8152	W	20001120 <--
	US 2002-150067	A1	20020520

OTHER SOURCE(S): MARPAT 134:367194
GI



I

AB Phenylalanine derivs. represented by general formula (I) or pharmaceutically acceptable salts thereof [wherein X represents an interat. bond, O, OSO2, N-(un)substituted NH, NHCO, NHSO2, NHCONH, or NH(CS)NH, CO; Y and Z represent each CO, SO, or SO2; A represents a specific substituted Ph group or nitrogen-containing heterocycle such as aromatic-fused pyrimidinedione or pyrimidinone, 2,4- or 2,5-imidazolidinedione, or 5-imidazolone; C represents hydrogen, lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally containing heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl; D and E represent each lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally containing heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl, etc. or D and E may be bonded to each other to form a ring optionally containing 1 or 2 O, N, or S in the ring; F and G represent each hydrogen, lower alkyl, lower alkenyl, lower alkynyl, cyclic alkyl-lower alkyl optionally containing heteroatoms in the ring, aryl-lower alkyl, heteroaryl-lower alkyl, etc. or F and G may be bonded to each other to form a ring; n is from 0 to 2; K represents OR7, NR7R8, NHNR7R8, SR7, or R7; R7 and R8 represents H, lower alkyl, etc.; and J and J' represent each hydrogen, halogeno, lower alkyl, lower alkoxy, or NO2] are prepared These derivs. and analogs thereof show an α4 integrin inhibitory activity and are usable as remedies for various diseases relating to α4 integrin, such as inflammatory diseases related to α4 integrin-dependent adhesion process, arthritis, inflammatory intestinal diseases, systemic lupus erythematosus, multiple sclerosis, Sjoegren syndrome, psoriasis, allergy, diabetes, cardiovascular diseases, arteriosclerosis, restenosis, ***tumor*** proliferation, ***tumor*** metastasis, or transplant rejection. Thus, O-(2,6-dichlorobenzyl)-L-tyrosine bound to Wang resin was allowed to react with diethylmalonic acid, HOAt, 2-dimethylaminoisopropyl chloride hydrochloride (DIC), and N-methyl-2-pyrrolidinone (NMP) at room temperature for 16 h, washed with DMF five times, and condensed with pyrroline using HOAt, DIC, and NMP, followed by oxidation with OsO4 in dioxane at room temperature for 16 and resin-cleavage in aqueous CF3CO2H to give N-[2-[(cis-2,4-dihydroxypyrrolidin-1-yl)carbonyl]-2-ethylbutanoyl]-O-(2,6-dichlorobenzyl)-L-tyrosine (II). II and N-[2-[(pyrrolidin-1-yl)carbonyl]-2-ethylbutanoyl]-4-(2,6-dichlorobenzoylamino)-L-phenylalanine inhibited the binding of human recombinant VCAM-1 to human B ***lymphoma*** cell line expressing integrinα4β7 with IC50 of ≤0.02 μmol/L.

IC C07C233-47; C07C233-63; C07C233-81; C07C275-42; C07C311-08; C07C311-21; C07C335-22; C07D295-18; C07D207-12; C07D211-62; C07D207-14; C07D207-16; C07D211-42; C07D211-46; C07D207-08; C07D487-08; C07D207-09; C07D265-30; C07D309-08; C07D211-22

CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1

ST phenylalanine deriv prepn integrin inhibitor; inflammatory disease

treatment phenylalanine deriv prepn; arthritis treatment phenylalanine deriv prepn; systemic lupus erythematosus treatment phenylalanine deriv prepn; multiple sclerosis treatment phenylalanine deriv prepn; Sjoegren syndrome treatment phenylalanine deriv prepn; psoriasis treatment phenylalanine deriv prepn; allergy treatment phenylalanine deriv prepn; diabetes treatment phenylalanine deriv prepn; cardiovascular disease treatment phenylalanine deriv prepn; arteriosclerosis treatment phenylalanine deriv prepn; restenosis treatment phenylalanine deriv prepn; *tumor* proliferation metastasis treatment phenylalanine deriv prepn; transplant rejection treatment phenylalanine deriv prepn; tyrosine deriv prepn integrin inhibitor

IT 340714-57-0P 340714-58-1P 340714-59-2P 340714-60-5P 340714-61-6P
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340717-23-9P ***340717-24-0P*** 340717-25-1P ***340717-26-2P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU

(Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel phenylalanine derivs. as α4-integrin inhibitors)

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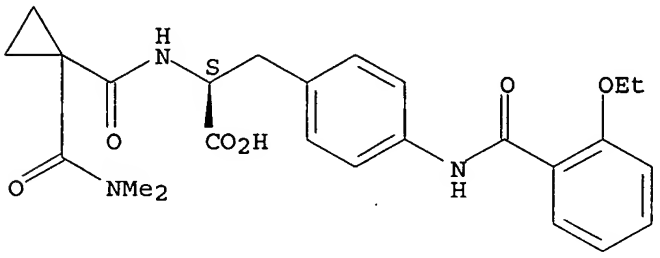
340719-68-8P 340719-69-9P 340719-70-2P 340719-71-3P 340719-72-4P
340719-73-5P 340719-74-6P 340719-76-8P 340719-77-9P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel phenylalanine derivs. as α4-integrin inhibitors)

IT ***340716-63-4P 340717-24-0P 340717-26-2P***
340717-62-6P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU

(Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel phenylalanine derivs. as α4-integrin inhibitors)

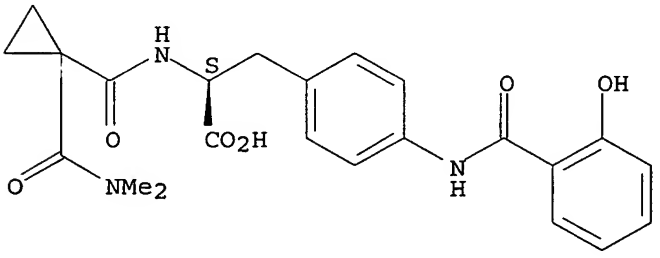
RN 340716-63-4 HCAPLUS
CN L-Phenylalanine, N-[[1-[(dimethylamino)carbonyl]cyclopropyl]carbonyl]-4-[(2-ethoxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



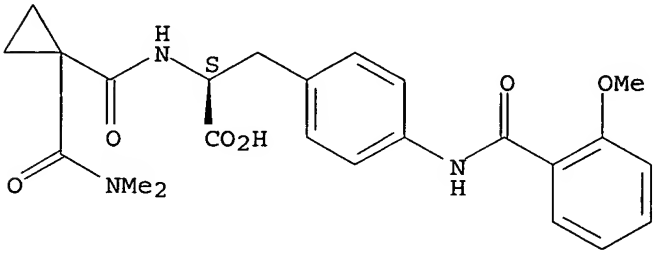
RN 340717-24-0 HCAPLUS
CN L-Phenylalanine, N-[[1-[(dimethylamino)carbonyl]cyclopropyl]carbonyl]-4-[(2-hydroxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 340717-26-2 HCAPLUS
CN L-Phenylalanine, N-[[1-[(dimethylamino)carbonyl]cyclopropyl]carbonyl]-4-[(2-methoxybenzoyl)amino]- (9CI) (CA INDEX NAME)

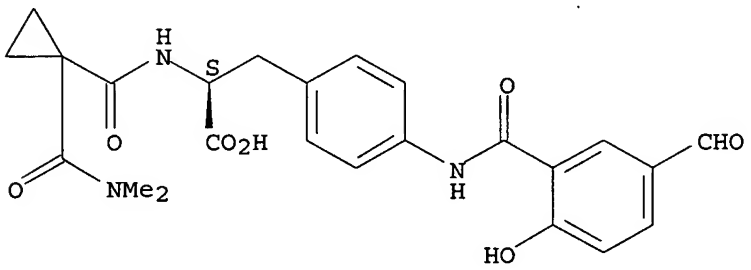
Absolute stereochemistry.



RN 340717-62-6 HCAPLUS

CN L-Phenylalanine, N-[[1-[(dimethylamino)carbonyl]cyclopropyl]carbonyl]-4-[(5-formyl-2-hydroxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 16 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:380396 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 135:500
TITLE: Benzene derivatives and use thereof as drugs
INVENTOR(S): Kaneeda, Masanobu; Sugawara, Yuji; Kawai, Hideki; Okano, Kiyoshi; Adachi, Yasumoto
PATENT ASSIGNEE(S): Toray Industries, Inc., Japan
SOURCE: PCT Int. Appl., 129 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001035955	A1	20010525	WO 2000-JP8058	20001116 <--

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: JP 1999-325207 A 19991116 <--

AB Benzene derivs. represented by general formula (I) or pharmacol. acceptable salts thereof; and drugs, particularly antihypocytotic agents, containing the derivs. or the salts as the active ingredient. The derivs. can induce the production of blood platelets, white blood cells, red blood cells, and so on, and are useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like.

IC ICM A61K031-12
ICS A61K031-216; A61K031-192; A61K031-167; A61K031-662; A61K031-381; A61K031-41; A61K031-37; A61K031-275; A61K031-235; A61K031-18; A61K031-661; C07C205-56; C07C049-84; C07C049-83; C07C059-90;

C07C205-45; C07C235-64; C07C317-24; C07C317-46
CC 1-8 (Pharmacology)
Section cross-reference(s): 8
IT Anemia (disease)
Antitumor agents
Erythrocyte
Leukocyte
Platelet (blood)
Radiotherapy
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)
IT Immunity
(disorder; benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)
IT 30865-93-1P 148930-79-4P 340959-72-0P 340959-74-2P 340959-75-3P
340959-77-5P 340959-80-0P 340959-81-1P 340959-83-3P 340959-84-4P
340959-99-1P 340960-00-1P 340960-06-7P 340960-08-9P 340960-11-4P
340960-12-5P 340960-22-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)
IT ***1152-51-8P*** 52122-86-8P 340959-70-8P 340959-71-9P
340959-73-1P 340959-76-4P 340959-78-6P 340959-79-7P 340959-82-2P
340959-85-5P 340959-86-6P 340959-87-7P 340959-88-8P 340959-89-9P
340959-90-2P 340959-91-3P 340959-92-4P 340959-93-5P 340959-94-6P
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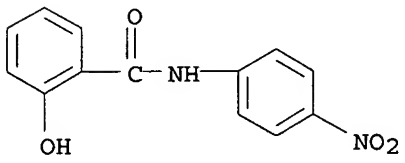
340960-27-2P 340960-28-3P 340960-29-4P 340960-55-6P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)
IT 50-78-2, Acetylsalicylic acid 100-01-6, p-Nitroaniline, reactions
104-92-7, 4-Bromoanisole 104-93-8, 4-Methoxytoluene 105-07-7,
4-Cyanobenzaldehyde 123-31-9, 1,4-Dihydroxybenzene, reactions
140-39-6, 4-Methylphenyl acetate 459-60-9, 4-Fluoroanisole 538-75-0,
1,3-Dicyclohexylcarbodiimide 830-03-5, p-Nitrophenyl acetate 872-50-4,
N-Methyl-2-pyrrolidinone, reactions 876-27-7, 4-Chlorophenyl acetate
1122-58-3, N,N-Dimethyl-4-aminopyridine 2100-42-7, 2,5-
Dimethoxychlorobenzene 5292-43-3, tert-Butyl bromoacetate 6341-97-5,
2,4-Dichlorophenyl acetate 13031-41-9, p-Cyanophenylacetate
24599-58-4, 2,5-Dimethoxytoluene 25245-34-5, 1-Bromo-2,5-
dimethoxybenzene 28165-71-1, 2,6-Dichlorophenyl acetate 39098-97-0,

2-Thiopheneacetyl chloride 50434-36-1 74426-51-0 90536-66-6
195609-18-8 287119-84-0 340960-30-7 340960-31-8 340960-32-9
340960-33-0 340960-37-4 340960-38-5 340960-39-6 340960-40-9
340960-41-0 340960-42-1 340960-44-3 340960-45-4 340960-47-6
340960-48-7 340960-50-1 340960-51-2 340960-52-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)

IT 25671-41-4P 74426-50-9P 82830-49-7P 340960-34-1P 340960-35-2P
340960-36-3P 340960-43-2P 340960-46-5P 340960-49-8P 340960-53-4P
340960-54-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)

IT ***1152-51-8P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(benzene derivs. and use thereof as drugs useful in chemotherapy of ***cancers***, radiotherapy or drug therapy and effective in the prevention or treatment of hypocytosis due to immune disorder, anemia or the like)

RN 1152-51-8 HCAPLUS
CN Benzamide, 2-hydroxy-N-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 17 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2001:78220 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 134:125939
TITLE: The use of retinoid receptor antagonists in the treatment of prostate carcinoma
INVENTOR(S): Chandraratna, Roshantha A.; Brown, Geoffrey
PATENT ASSIGNEE(S): Allergan Sales, Inc., USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2001007028	A2	20010201	WO 2000-US19849	20000721 <--
WO 2001007028	A3	20010830		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 1999-145287P P 19990723 <--

OTHER SOURCE(S): MARPAT 134:125939

AB Methods for treating prostate ***cancer*** comprise administering a therapeutically effective amount of a retinoid receptor antagonist. In addition, the invention provides methods of inhibiting the growth of a prostate carcinoma cell or ***tumor***, the method comprising contacting the cell or ***tumor*** with an effective amount of a retinoid receptor antagonist.

IC ICM A61K031-00

CC 1-6 (Pharmacology)
Section cross-reference(s): 63

ST ***cancer*** prostate treatment retinoid receptor antagonist; carcinoma prostate treatment retinoid receptor antagonist

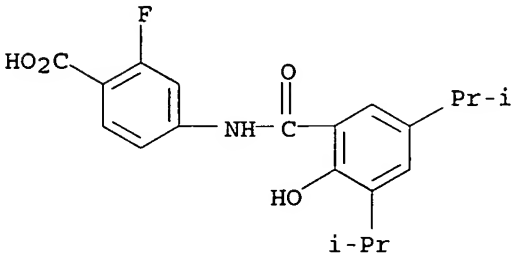
IT Prostate gland
(***neoplasm***, inhibitors; retinoid receptor antagonist for treatment of prostate carcinoma)

IT 302-79-4, all-trans-Retinoic acid 118292-40-3, AGN 190168 118292-41-4, AGN 190299 260262-39-3, AGN 194204 321995-62-4, AGN 194078 ***321995-64-6***, AGN 194365 321995-65-7, AGN 195153
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); BIOL (Biological study)
(retinoid receptor antagonist for treatment of prostate carcinoma)

IT ***321995-64-6***, AGN 194365
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); BIOL (Biological study)
(retinoid receptor antagonist for treatment of prostate carcinoma)

RN 321995-64-6 HCAPLUS

CN Benzoic acid, 2-fluoro-4-[[2-hydroxy-3,5-bis(1-methylethyl)benzoyl]amino]- (9CI) (CA INDEX NAME)

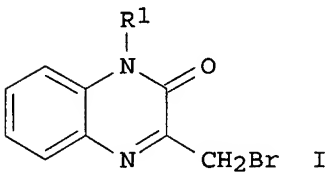


L101 ANSWER 18 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN

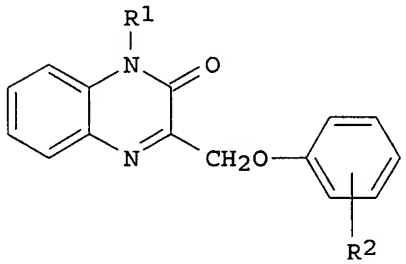
ACCESSION NUMBER: 2001:31481 HCAPLUS <<LOGINID::20061006>>

DOCUMENT NUMBER: 134:100859

ACCESSION NUMBER: 2000:897082 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 134:207794
TITLE: Structure-activity studies of substituted quinoxalinones as multiple-drug-resistance antagonists
AUTHOR(S): Lawrence, David S.; Copper, Jean E.; Smith, Charles D.
CORPORATE SOURCE: Department of Pharmacology, Pennsylvania State University, Hershey, PA, 17033, USA
SOURCE: Journal of Medicinal Chemistry (*2001*), 44(4), 594-601
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB A significant problem in the clin. treatment of ***cancer*** relates to the development of ***tumor*** resistance to many chemotherapeutic agents. Acquired drug resistance is often mediated through overexpression of membrane transport proteins that effectively efflux ***anticancer*** agents. Two of the best-studied transporters, P-glycoprotein (Pgp) and MRP1, have pharmacol. properties that only partially overlap. In the search for improved drug-resistance antagonists, the authors have identified a family of substituted quinoxalines that selectively antagonizes Pgp over MRP1. A focused library of congeners was designed and synthesized starting with a parent (bromomethyl)quinoxalinone. This parent quinoxalinone, I (R1 = Me, PhCH2), was then condensed with a series of phenols R2C6H4OH (R2 = H, 4-F, 4-CN, 3-t-Bu, 3,4-Cl2, 2-PhNHCO, etc.) and 3-hydroxypyridine to yield a family of substituted (phenoxymethyl)quinoxalinones II. These compds. were evaluated for their toxicity toward drug-sensitive MCF-7 breast carcinoma cells and for their abilities to antagonize Pgp and MRP1 in drug-resistant cell lines (NCI/ADR and MCF-7/VP, resp.). The results of this structure-activity study indicate that compds. with carbonyl substitutions of the phenoxy group (ester, amide, or ketone moieties) demonstrate excellent antagonism of Pgp while having relatively low toxicity toward drug-sensitive cells. Importantly, none of these compds. antagonized MRP1. Because of the transporter selectivity of the substituted quinoxalinones, the authors predict that they may be more effective MDR modulators in vivo than are nonselective transporter antagonists.

CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

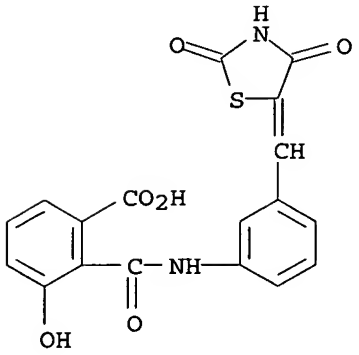
ST structure multidrug resistance antagonist quinoxalinone; cytotoxicity quinoxalinone prepn; ***anticancer*** quinoxalinone prepn

IT 24949-43-7P 132346-18-0P 328249-91-8P 328249-92-9P 328249-93-0P

ylidenemethyl)phenoxy]benzenesulfonamide 319454-37-0P, N-(3-Chlorophenyl)-4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]benzenesulfonamide 319454-38-1P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(4-hydroxyphenyl)benzenesulfonamide 319454-39-2P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(2-hydroxyphenyl)benzenesulfonamide 319454-40-5P, N-(2-tert-Butylphenyl)-4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]benzenesulfonamide 319454-41-6P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-isopropyl-N-phenylbenzenesulfonamide 319454-42-7P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(3-hydroxyphenyl)benzenesulfonamide 319454-43-8P, 5-[3-Amino-2-(2,4-dichlorobenzoyl)thieno[2,3-b]pyridin-6-ylmethylene]thiazolidine-2,4-dione 319454-44-9P, 2-Chloro-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-45-0P, 2-Phenylthio-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-47-2P, 2-(3,4-Dichlorophenylthio)-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-48-3P, 2-(4-Fluorophenylthio)-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-49-4P, 2-(4-Methylphenylthio)-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-50-7P, 2-(4-Methoxyphenylthio)-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-51-8P, 2-[4-Trifluoromethylphenylthio]-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline 319454-52-9P, 2-(4-Chlorophenylsulfinyl)-3-(2,4-dioxothiazolidin-5-ylidenemethyl)quinoline
RL: SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity and methods of use)

IT ***319454-19-8P***, N-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenyl]-3-hydroxyphthalamic acid
RL: SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity and methods of use)

RN 319454-19-8 HCAPLUS
CN Benzoic acid, 2-[[[3-[(2,4-dioxo-5-thiazolidinylidene)methyl]phenyl]amino]carbonyl]-3-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 19 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN

methylphenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-91-3P, 5-((2-(4-Methylphenylthio)-5-(4-morpholinecarbonyl)phenyl)methylene)-2,4-thiazolidinedione 319453-96-8P, 5-((2-(2,3-Dichlorophenylsulfinyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-97-9P, 5-((2-(2,4-Dichlorophenylsulfinyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-98-0P, 5-((2-(2,3-Dichlorophenylsulfonyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-99-1P, 5-((2-(2,4-Dichlorophenylsulfonyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-00-7P, 5-((2-(4-Hydroxyphenylthio)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-02-9P, 5-((2-(3,4-Dichlorophenylsulfonyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-03-0P, 5-((4-(4-Chlorophenylsulfinyl)-3-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-05-2P, 5-((4-(4-Ethylphenylsulfinyl)-3-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-06-3P, 5-((2-(4-Ethylphenylsulfonyl)-3-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-08-5P, 5-((4-(3,4-Dichlorophenylsulfinyl)-3-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-09-6P, 5-((2-(2,3-Dimethylphenylsulfinyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-10-9P, 5-((2-(2,3-Dimethylphenylsulfonyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319454-12-1P, N-(4-Chlorophenyl)-4-(2,4-dioxothiazolidin-5-ylidenemethyl)benzenesulfonamide 319454-13-2P, 4-(2,4-Dioxothiazolidin-5-ylidenemethyl)-N-p-tolylbenzenesulfonamide 319454-14-3P, 4-(2,4-Dioxothiazolidin-5-ylidenemethyl)-N-(4-methoxyphenyl)benzenesulfonamide 319454-15-4P, 4-(2,4-Dioxothiazolidin-5-ylidenemethyl)-N-(4-trifluoromethylphenyl)benzenesulfonamide 319454-16-5P, 4,5-Dichloro-N-[3-(2,4-dioxothiazolidin-5-ylidenemethyl)phenyl]phthalamic acid 319454-17-6P, 3,6-Dichloro-N-[3-(2,4-dioxothiazolidin-5-ylidenemethyl)phenyl]phthalamic acid 319454-18-7P, 4-tert-Butyl-N-[3-(2,4-dioxothiazolidin-5-ylidenemethyl)phenyl]phthalamic acid ***319454-19-8P***, N-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenyl]-3-hydroxyphthalamic acid 319454-20-1P, 3-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenylcarbamoyl]pyrazine-2-carboxylic acid 319454-21-2P, 3-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenylcarbamoyl]isonicotinic acid 319454-22-3P, 3-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenylcarbamoyl]pyridine-2-carboxylic acid 319454-23-4P, 4-(4-Chlorobenzenesulfonylamino)-N-[3-(2,4-dioxothiazolidin-5-ylidenemethyl)phenyl]benzamide 319454-24-5P, N-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenyl]-4-(toluene-4-sulfonylamino)benzamide 319454-25-6P, N-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenyl]-4-(4-methoxybenzenesulfonylamino)benzamide 319454-26-7P, N-[3-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenyl]-4-(4-trifluoromethoxybenzenesulfonylamino)benzamide 319454-27-8P, 4-Benzenesulfonylamino-N-[3-(2,4-dioxothiazolidin-5-ylidenemethyl)phenyl]benzamide 319454-28-9P, N-(4-Chlorophenyl)-4-[4-(2,4-dioxothiazolidin-5-ylidenemethyl)phenoxy]benzenesulfonamide 319454-29-0P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-p-tolylbenzenesulfonamide 319454-30-3P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(4-trifluoromethoxyphenyl)benzenesulfonamide 319454-31-4P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(4-methoxyphenyl)benzenesulfonamide 319454-32-5P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-phenylbenzenesulfonamide 319454-33-6P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(3,4,5-trimethoxyphenyl)benzenesulfonamide 319454-34-7P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(4-morpholin-4-ylphenyl)benzenesulfonamide 319454-35-8P, 4-[4-(2,4-Dioxothiazolidin-5-ylidenemethyl)phenoxy]-N-(4-isopropylphenyl)benzenesulfonamide 319454-36-9P, N-(2-Chlorophenyl)-4-[4-(2,4-dioxothiazolidin-5-

dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319452-26-1P, 5-(2-(3,4-Dichlorophenoxy)benzylidene)thiazolidine-2,4-dione 319452-27-2P, 5-(4-(3,4-Dichlorophenoxy)benzylidene)thiazolidine-2,4-dione 319452-28-3P, 5-(2,5-Bis(3,4-dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319452-30-7P, 5-(2,4-Bis(3,4-dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319452-32-9P, 5-(2-(3,4-Dichlorobenzylthio)-3H-pyrimidin-4-on-6-ylmethylidene)rhodanine 319452-33-0P, 5-(2-(3,4-Dichlorobenzylthio)pyrimidin-4-ylmethylidene)rhodanine 319452-34-1P, 5-[2-(3,4-Dichlorobenzylthio)pyrimidin-4-ylmethyl]-2-thioxothiazolidin-4-one 319452-35-2P, 5-(3-Cyano-2-(3,4-dichlorobenzylthio)pyridin-6-ylmethylidene)thiazolidine-2,4-dione 319452-36-3P, 5-(3-(3,4-Dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319452-42-1P, 5-((2-(4-Chlorophenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319452-43-2P, 5-((2-Phenoxyphenyl)methylene)-2,4-thiazolidinedione 319452-49-8P, 5-((4-(4-Methylphenoxy)phenyl)methylene)-2,4-thiazolidinedione 319452-56-7P, 5-((4-(Bis(4-bromophenyl)amino)phenyl)methylene)-2,4-thiazolidinedione 319452-61-4P, 5-((2-(Benzyl(4-bromophenyl)amino)phenyl)methylene)-2,4-thiazolidinedione 319452-70-5P, 5-((2-Phenylphenyl)methylene)-2,4-thiazolidinedione 319452-72-7P, 5-((3-Phenylphenyl)methylene)-2,4-thiazolidinedione 319452-73-8P, 5-((4-Phenylphenyl)methylene)-2,4-thiazolidinedione 319452-80-7P, 5-((4-(Diphenylmethyl)phenyl)methylene)-2,4-thiazolidinedione 319452-84-1P, 5-((5-Nitro-2-(4-(trifluoromethyl)phenoxy)phenyl)methylene)-2,4-thiazolidinedione 319452-85-2P, 5-((2-Bromo-5-((4-tolyl)methoxy)phenyl)methylene)-2,4-thiazolidinedione 319452-86-3P, 5-((2,5-Bis((4-Tolyl)methoxy)phenyl)methylene)-2,4-thiazolidinedione 319452-87-4P, 5-(1-(5-Bromo-2-((4-tolyl)methoxy)phenyl)ethylidene)-2,4-thiazolidinedione 319452-90-9P, 5-((2-(4-Chlorophenylthio)-3-thienyl)methylene)-2,4-thiazolidinedione 319452-91-0P, 5-((5-Bromo-2-(4-chlorophenylsulfinyl)-3-thienyl)methylene)-2,4-thiazolidinedione 319452-92-1P, 5-((5-Bromo-2-(4-chlorophenylsulfonyl)-3-thienyl)methylene)-2,4-thiazolidinedione 319453-17-3P, 5-((5-Nitro-2-(phenylmethylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-25-3P, 5-((2-Cyclohexylsulfinyl-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-38-8P, 5-((5-Acetyl-2-(4-methylphenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-43-5P, 5-((2-(4-Methylphenylsulfinyl)-3-(trifluoromethyl)phenyl)methylene)-2,4-thiazolidinedione 319453-45-7P, 5-((4-Methoxy-2-(4-methylphenylthio)phenyl)methylene)-2,4-thiazolidinedione 319453-47-9P, 5-((5-Chloro-2-(4-methylphenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-51-5P, 5-((2-(4-Methylphenoxy)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-52-6P, 5-((2-(4-Isobutylphenoxy)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-54-8P, 5-((5-Cyano-2-(4-methylphenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-56-0P, 5-((2-(4-Methoxyphenylsulfinyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-57-1P, 5-((2-(2-Chlorophenylsulfinyl)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-70-8P, 5-((2-(4-(Dimethylcarbamoyl)phenylthio)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-71-9P, 5-((2-(4-(4-Morpholinecarbonyl)phenylthio)-5-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-76-4P, 5-((4-(4-Bromophenylsulfinyl)-3-nitrophenyl)methylene)-2,4-thiazolidinedione 319453-80-0P, 5-((3-Cyano-4-(4-methylphenylsulfinyl)phenyl)methylene)-2,4-thiazolidinedione 319453-86-6P, 5-((5-(3-Hydroxy-3-oxo-1-propenyl)-2-(4-methylphenylthio)phenyl)methylene)-2,4-thiazolidinedione 319453-88-8P, 5-((4-(4-Methylphenylsulfinyl)-3-(trifluoromethyl)phenyl)methylene)-2,4-thiazolidinedione 319453-90-2P, 5-((5-Diethylcarbamoyl-2-(4-

AB Thiazolidinedione compds. (shown as I; e.g. 5-((2-(4-chlorophenylthio)-5-nitrophenyl)methylene)-2,4-thiazolidinedione), compns., and methods of inhibiting telomerase activity in vitro and treatment of telomerase-mediated conditions or diseases ex vivo and in vivo are provided. In I, X = O or S; the dashed bond is a single or double bond; A = aryl or heteroaryl; R1 = H or lower alkyl; R2, R3 and R4 are independently selected from H, halo, alkyl, aryl, hydroxyl, alkoxyl, aryloxy, aralkoxy, cyano, nitro, alkylcarbamido, arylcarbamido, dialkylcarbamido, diarylcarbamido, alkylarylcarbamido, alkylthiocarbamido, arylthiocarbamido, dialkylthiocarbamido, diarylthiocarbamido, alkylarylthiocarbamido, amino, alkylamino, arylamino, dialkylamino, diarylamino, arylalkylamino, aminocarbonyl, alkylaminocarbonyl, arylaminocarbonyl, dialkylaminocarbonyl, diarylaminocarbonyl, arylalkylaminocarbonyl, alkylcarbonyloxy, arylcarbonyloxy, carboxyl, alkoxycarbonyl, aryloxycarbonyl, sulfo, alkylsulfonylamido, arylsulfonylamido, alkylsulfonyl, arylsulfonyl, alkylsulfinyl, arylsulfinyl and heteroaryl; L is a direct bond or a linking group having from 1 to 3 unsubstituted or substituted C, N, O or S atoms; and n = 1, 2. A pharmaceutically acceptable salt thereof is also claimed. The methods, compds. and compns. of the invention may be employed alone, or in combination with other pharmacol. active agents in the treatment of conditions or diseases mediated by telomerase activity, such as in the treatment of ***cancer***. Also disclosed are novel methods for assaying or screening for inhibitors of telomerase activity. More than 200 example prepns. are included, but the methods of preparation are not claimed.

IC ICM C07D277-34
ICS C07D277-36; C07D417-06; C07D417-10; C07D513-04; A61K031-425; A61K031-44

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7

ST telomerase inhibitor dioxothiazolidine oxothioxothiazolidine prepn activity; thiazolidine dioxo oxothioxo prepn telomerase inhibition; ***cancer*** treatment dioxothiazolidine oxothioxothiazolidine telomerase inhibition

IT 319451-93-9P, 5-(2-(3,4-Dichlorophenyl)benzylidene)thiazolidine-2,4-dione 319451-95-1P, 5-(3-(3,4-Dichlorophenyl)benzylidene)thiazolidine-2,4-dione 319451-97-3P, 5-(4-(3,4-Dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319451-99-5P, 5-(2-(3,4-Dichlorobenzyloxy)benzylidene)thiazolidine-2,4-dione 319452-00-1P, 5-(4-(3,4-Dichlorobenzamido)benzylidene)thiazolidine-2,4-dione 319452-02-3P, 5-(4-(N-3,4-Dichlorophenylureido)benzylidene)thiazolidine-2,4-dione 319452-04-5P, 5-(2-(N-3,4-Dichlorophenylureido)benzylidene)thiazolidine-2,4-dione 319452-06-7P, 5-(2-(3,4-Dichlorophenylcarbamoyl)benzylidene)thiazolidine-2,4-dione 319452-08-9P, 5-(3-(3,4-Dichlorophenylcarbamoyl)benzylidene)thiazolidine-2,4-dione 319452-10-3P, 5-(4-(3,4-Dichlorophenylcarbamoyl)benzylidene)thiazolidine-2,4-dione 319452-12-5P, 5-(4-(N-3,4-Dichlorophenylcarbamoyloxy)benzylidene)thiazolidine-2,4-dione 319452-13-6P, 5-(4-(3,4-Dichlorophenoxycarbonyl)benzylidene)thiazolidine-2,4-dione 319452-14-7P, 5-(2-(3,4-Dichlorophenoxycarbonyl)benzylidene)thiazolidine-2,4-dione 319452-16-9P, 5-(2-(3,4-Dichlorophenylacetoxy)benzylidene)thiazolidine-2,4-dione 319452-18-1P, 5-(3-(3,4-Dichlorophenylacetoxy)benzylidene)thiazolidine-2,4-dione 319452-20-5P, 5-(4-(3,4-Dichlorophenylacetoxy)benzylidene)thiazolidine-2,4-dione 319452-21-6P, 5-(2-(3,4-Dichlorobenzoyloxy)benzylidene)thiazolidine-2,4-dione 319452-22-7P, 5-(3-(3,4-Dichlorobenzoyloxy)benzylidene)thiazolidine-2,4-dione 319452-23-8P, 5-(4-(3,4-Dichlorobenzoyloxy)benzylidene)thiazolidine-2,4-dione 319452-24-9P, 5-(3,4-Bis(3,4-

TITLE: Preparation of 2,4-dioxothiazolidines and 4-oxo-2-thioxothiazolidines having telomerase inhibitory activity and methods of their use

INVENTOR(S): Chin, Allison C.; Holcomb, Ryan; Piatyszek, Mieczyslaw A.; Singh, Upinder; Tolman, Richard L.; Akama, Tsutomu; Kanda, Yutaka; Asai, Akira; Yamashita, Yoshinori; Endo, Kaori; Yamaguchi, Hiroyuki

PATENT ASSIGNEE(S): Geron Corporation, USA; Kyowa Hakko Kogyo Co., Ltd.

SOURCE: PCT Int. Appl., 211 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001002377	A1	20010111	WO 2000-US18211	20000630 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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JP 2001072592	A2	20010321	JP 1999-307576	19991028 <--
CA 2341253	AA	20010111	CA 2000-2341253	20000630 <--
EP 1109796	A1	20010627	EP 2000-950282	20000630 <--
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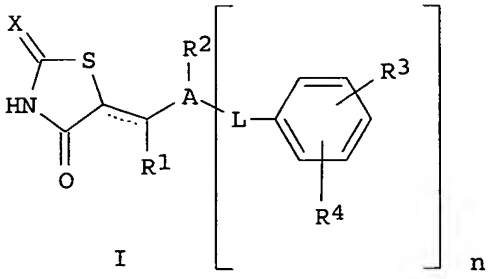
JP 2003507473	T2	20030225	JP 2001-518671	20000630 <--
US 2002115700	A1	20020822	US 2002-77738	20020213 <--

PRIORITY APPLN. INFO.:

JP 1999-187616	A	19990701 <--
US 1999-142173P	P	19990701 <--
JP 1999-307576	A	19991028 <--
US 2000-608861	A1	20000630 <--
WO 2000-US18211	W	20000630 <--

OTHER SOURCE(S): MARPAT 134:100859

GI



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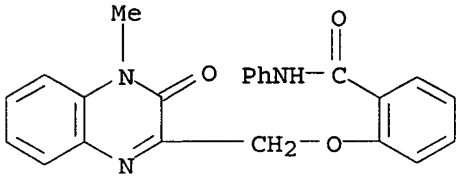
328249-94-1P 328249-95-2P 328249-96-3P 328249-97-4P 328249-98-5P
328249-99-6P 328250-00-6P ***328250-01-7P*** 328250-02-8P
328250-03-9P 328250-04-0P 328250-05-1P 328250-06-2P 328250-07-3P
328250-08-4P 328250-09-5P 328250-10-8P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, antitumor activity, multiple-drug resistance antagonist activity, and structure-activity relationship of quinoxalinones)

IT ***87-17-2*** 90-15-3, 1-Naphthalenol 92-69-3, 4-Phenylphenol 95-54-5, 1,2-Benzenediamine, reactions 95-77-2 99-07-0, 3-(Dimethylamino)phenol 101-18-8 103-16-2, 4-Benzyloxyphenol 108-95-2, Phenol, reactions 109-00-2, 3-Hydroxypyridine 120-47-8 127-17-3, reactions 135-19-3, 2-Naphthalenol, reactions 156-06-9 371-41-5, 4-Fluorophenol 585-34-2, 3-tert-Butylphenol 767-00-0, 4-Hydroxybenzonitrile 771-61-9 1137-42-4, 4-Benzoylphenol 2581-34-2 3943-74-6 4760-34-3 28994-41-4, 2-Benzylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, antitumor activity, multiple-drug resistance antagonist activity, and structure-activity relationship of quinoxalinones)

IT ***328250-01-7P 328250-08-4P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, antitumor activity, multiple-drug resistance antagonist activity, and structure-activity relationship of quinoxalinones)

RN 328250-01-7 HCAPLUS
CN Benzamide, 2-[(3,4-dihydro-4-methyl-3-oxo-2-quinoxalinyl)methoxy]-N-phenyl- (9CI) (CA INDEX NAME)



RN 328250-08-4 HCAPLUS
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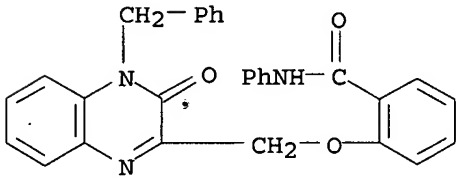
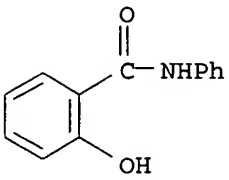


IT ***87-17-2***
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, antitumor activity, multiple-drug resistance antagonist

activity, and structure-activity relationship of quinoxalinones)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 20 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:688014 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 133:256832
TITLE: Oral low dose butyrate compositions
INVENTOR(S): Chaturvedi, Pravin; Su, Michael; Tung, Roger
PATENT ASSIGNEE(S): Vertex Pharmaceuticals Incorporated, USA
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000056153	A1	20000928	WO 2000-US7128	20000317 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2366650	AA	20000928	CA 2000-2366650	20000317 <--
EP 1162884	A1	20011219	EP 2000-916478	20000317 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002539227	T2	20021119	JP 2000-606071	20000317 <--
US 2002115716	A1	20020822	US 2001-955707	20010919 <--
PRIORITY APPLN. INFO.:			US 1999-125607P P	19990319 <--
			WO 2000-US7128 W	20000317 <--

AB This invention relates to orally available compns. which deliver an amount of butyrate or a butyrate analog effective to ameliorate β-hemoglobinopathies, such as β-thalassemia and sickle cell anemia, cystic fibrosis, ***cancer*** and other diseases which are known to be treatable with butyrate. The invention also relates to methods of treating these diseases with such low dose oral compns.
IC ICM A01N037-10
ICS A01N037-18; A01N025-00; A61K031-235; A61K031-165; A61K047-00
CC 63-6 (Pharmaceuticals)

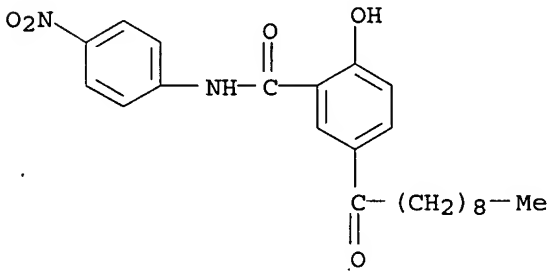
Section cross-reference(s): 1

IT 60-01-5, Tributyrin 107-92-6D, Butyric acid, salts or analogs or prodrugs 1821-12-1, Benzenebutanoic acid 7631-42-7, Phenyl acetate, biological studies ***78417-88-6***, AN-10 122110-53-6, AN-9 296228-84-7
RL: ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(oral low dose butyrate compns.)

IT ***78417-88-6***, AN-10
RL: ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(oral low dose butyrate compns.)

RN 78417-88-6 HCAPLUS

CN Benzamide, 2-hydroxy-N-(4-nitrophenyl)-5-(1-oxodecyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 21 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:117019 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 132:166015
TITLE: Preparation of benzamides as cytokine inhibitors
INVENTOR(S): Brown, Dearg Sutherland; Brown, George Robert
PATENT ASSIGNEE(S): Zeneca Ltd., UK
SOURCE: PCT Int. Appl., 110 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000007980	A1	20000217	WO 1999-GB2494	19990729 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2337770	AA	20000217	CA 1999-2337770	19990729 <--
AU 9951791	A1	20000228	AU 1999-51791	19990729 <--
AU 756292	B2	20030109		
BR 9912726	A	20010502	BR 1999-12726	19990729 <--

EP 1102743	A1	20010530	EP 1999-936814		19990729 <--
EP 1102743	B1	20020724			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002522414	T2	20020723	JP 2000-563615		19990729 <--
AT 221047	E	20020815	AT 1999-936814		19990729 <--
PT 1102743	T	20021231	PT 1999-936814		19990729 <--
ES 2178895	T3	20030101	ES 1999-936814		19990729 <--
RU 2220951	C2	20040110	RU 2001-105984		19990729 <--
NZ 509162	A	20040130	NZ 1999-509162		19990729 <--
ZA 2001000617	A	20020122	ZA 2001-617		20010122 <--
NO 2001000533	A	20010330	NO 2001-533		20010131 <--
NO 321017	B1	20060227			
US 6821965	B1	20041123	US 2001-762106		20010202 <--
HK 1037608	A1	20021129	HK 2001-108406		20011129 <--
US 2005038081	A1	20050217	US 2004-947463		20040923 <--
PRIORITY APPLN. INFO.:			GB 1998-16837	A	19980804 <--
			WO 1999-GB2494	W	19990729 <--
			US 2001-762106	A3	20010202 <--

OTHER SOURCE(S): MARPAT 132:166015

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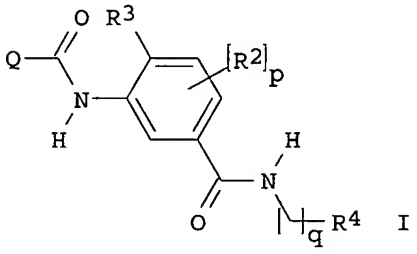

I

AB The title compds. [I; R3 = alkyl, halo; Q = (un)substituted aryl, heteroaryl; p = 0-2; R2 = OH, halo; q = 0-4; R4 = (un)substituted aryl, cycloalkyl, heteroaryl, heterocyclyl], useful in the treatment of diseases or medical conditions mediated by cytokines, were prepared and formulated. Thus, reacting 3-amino-N-(3-dimethylaminophenyl)-4-methylbenzamide (preparation given) with 3-methoxybenzoyl chloride in the presence of Et3N in CH2Cl2 afforded I [Q = 3-MeOC6H4; p = 0; R3 = Me; R4 = 3-Me2NC6H4; q = 0]. Biol. data (e.g., inhibition of p38 kinase and TNFα production) for compds. I were presented.

IC ICM C07C237-42
ICS C07D295-12; C07D295-14; C07D213-82; C07D215-48; A61K031-167; A61K031-395

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 28, 63

ST benzamide prepn cytokine inhibitor; p38 kinase inhibitor benzamide prepn; ***tumor*** necrosis factor alpha prodn inhibitor benzamide prepn; TNF alpha prodn inhibitor benzamide prepn; amide prepn cytokine inhibitor

IT ***Tumor*** necrosis factors
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of benzamides as cytokine inhibitors)

IT 258862-54-3P 258862-55-4P 258862-56-5P 258862-57-6P 258862-58-7P
258862-59-8P 258862-60-1P 258862-61-2P 258862-62-3P 258862-63-4P

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258862-69-0P 258862-70-3P 258862-71-4P 258862-72-5P 258862-73-6P
258862-74-7P 258862-75-8P 258862-76-9P 258862-77-0P 258862-78-1P
258862-81-6P 258862-85-0P 258862-87-2P 258862-90-7P 258862-92-9P
258862-95-2P 258862-96-3P 258862-97-4P ***258862-98-5P***
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258863-24-0P 258863-25-1P 258863-26-2P 258863-27-3P 258863-28-4P
258863-29-5P 258863-30-8P 258863-31-9P 258863-32-0P 258863-33-1P
258863-34-2P 258863-35-3P 258863-36-4P 258863-37-5P 258863-38-6P
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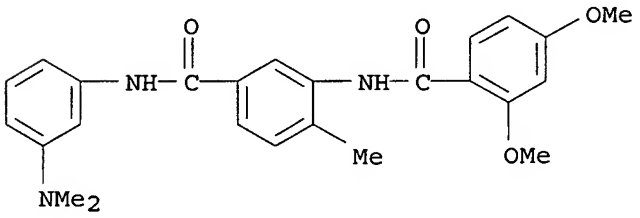
258863-70-6P 258863-71-7P 258863-72-8P 258863-73-9P 258863-74-0P
258863-75-1P 258863-76-2P 258863-77-3P 258863-79-5P 258863-80-8P
258863-81-9P 258863-82-0P 258863-83-1P 258863-84-2P 258863-85-3P
258863-86-4P 258863-87-5P 258863-88-6P 258863-89-7P 258863-90-0P
258863-91-1P 258863-92-2P 258863-93-3P 258863-94-4P 258863-95-5P
258863-96-6P 258863-97-7P 258863-98-8P 258863-99-9P 258864-00-5P
258864-01-6P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzamides as cytokine inhibitors)

IT ***258862-98-5P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzamides as cytokine inhibitors)

RN 258862-98-5 HCAPLUS
CN Benzamide, N-[5-[[[3-(dimethylamino)phenyl]amino]carbonyl]-2-methylphenyl]-2,4-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 22 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:205323 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 130:267221

TITLE: Preparation of phenylureas as IL-8 receptor antagonists
INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Hertzberg, Robert Phillip; Rutledge, Melvin Clarence, Jr.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 43 pp., Cont.-in-part of U.S. Ser. No. 390,260, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5886044	A	19990323	US 1996-641990	19960320 <--
US 5780483	A	19980714	US 1996-701299	19960821 <--
US 6211373	B1	20010403	US 1998-111663	19980708 <--
US 6262113	B1	20010717	US 1998-125279	19980814 <--
US 6180675	B1	20010130	US 1999-240354	19990129 <--

PRIORITY APPLN. INFO.:
US 1995-390260 B2 19950217 <--
WO 1996-US2260 W 19960216 <--
US 1996-641990 A2 19960320 <--
US 1996-701299 A3 19960821 <--
WO 1996-US13632 W 19960821 <--

OTHER SOURCE(S): MARPAT 130:267221
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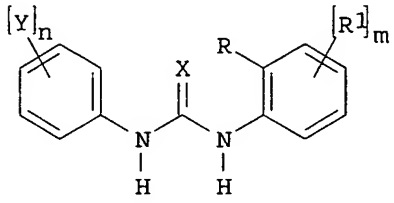


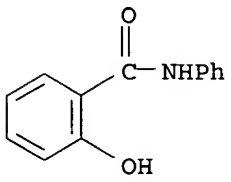
I

AB The title compds. [I; X = O, S; R = OH; R1 = H, halo, NO2, etc.; Y = H, halo, CN, etc.; n = 1-3; m = 1-3], useful in the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8), such as psoriasis, atopic dermatitis, ***asthma***, chronic obstructive pulmonary disease, ARDS, arthritis, inflammatory bowel disease, Crohn's disease, ulcerative colitis, septic shock, toxic shock syndrome, stroke, cardiac and renal reperfusion injury, restenosis, angiogenesis, glomerulonephritis, thrombosis, Alzheimer's disease, graft vs. host reaction, allograft rejection, etc., were prepared E.g., reaction of Me 4-amino-3-hydroxybenzoate with Ph isocyanate afforded 90% I [R = OH; R1 = 4-(MeOCO); Y = H; m = 1]. All exemplified compds. I showed IC50 from 45 to <1 μ/mL for IL-8 receptor inhibition. Compds. I were also found to be inhibitors of Gro-α binding at about the same level.
IC ICM A61K031-17
INCL 514596000
CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
IT 62-53-3, Aniline, reactions 86-84-0, 1-Naphthyl isocyanate

87-17-2, 2-Phenylaminocarbonylphenol 88-67-5, 2-Iodobenzoic acid
90-43-7, 2-Phenylphenol 91-93-0 95-54-5, 1,2-Benzenediamine, reactions
95-55-6, 2-Aminophenol 98-09-9, Phenylsulfonyl chloride 98-17-9
99-56-9, 4-Nitro-1,2-phenylenediamine 99-57-0, 5-Nitro-2-hydroxyaniline
100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions
106-40-1, 4-Bromoaniline 116-63-2 117-77-1, 2-Hydroxy-3-
aminoanthraquinone 117-99-7 121-51-7, 3-Nitrobenzenesulfonyl chloride
121-60-8, 4-Acetamidophenylsulfonyl chloride 121-88-0,
2-Amino-5-nitrophenol 137-07-5, 2-Aminothiophenol 274-09-9,
1,3-Benzodioxole 320-76-3 329-01-1, 3-Trifluoromethylphenyl isocyanate
385-01-3, 2-Nitro-3-fluorophenol 394-31-0, 2-Amino-5-hydroxybenzoic acid
394-33-2, 4-Fluoro-2-nitrophenol 400-98-6, 4-Amino-3-
nitrobenzotrifluoride 400-99-7, 4-Trifluoromethyl-2-nitrophenol
444-30-4, 2-Trifluoromethylphenol 446-36-6, 5-Fluoro-2-nitrophenol
534-85-0, 2-Anilinoaniline 570-23-0, 2-Hydroxy-3-aminobenzoic acid
576-24-9, 2,3-Dichlorophenol 580-51-8, 3-Phenylphenol 583-17-5,
2-Hydroxycinnamic acid 588-30-7, 3-Hydroxycinnamic acid 603-87-2,
2-Hydroxy-3-nitroaniline 609-89-2, 4,6-Dichloro-2-nitrophenol
611-20-1, 2-Cyanophenol 614-68-6, 2-Methylphenyl isocyanate 615-36-1,
2-Bromoaniline 618-45-1, 3-Isopropylphenol 620-17-7, 3-Ethylphenol
644-35-9, 2-n-Propylphenol 700-38-9, 2-Nitro-5-methylphenol 700-87-8,
2-Methoxyphenyl isocyanate 776-04-5, 2-(Trifluoromethyl)benzenesulfonyl
chloride 837-95-6, 2-Nitro-4-trifluoromethylbenzenesulfonyl chloride
873-62-1, 3-Cyanophenol 1548-13-6, 4-Trifluoromethylphenyl isocyanate
1592-00-3, 2-Bromophenyl isocyanate 1623-92-3, 4-Phenoxyphenylsulfonyl
chloride 1899-93-0 1939-99-7, Benzylsulfonyl chloride 2237-30-1,
3-Cyanoaniline 2243-42-7, 2-Phenoxybenzoic acid 2285-12-3,
2-Trifluoromethylphenyl isocyanate 2374-03-0, 3-Hydroxy-4-aminobenzoic
acid 2493-02-9, 4-Bromophenyl isocyanate 2612-57-9, 2,4-Dichlorophenyl
isocyanate 2834-92-6, 1-Amino-2-hydroxynaphthalene 2835-98-5,
2-Hydroxy-4-methylaniline 3272-08-0, 2-Nitro-4-cyanophenol 3320-83-0,
2-Chlorophenyl isocyanate 3320-86-3, 2-Nitrophenyl isocyanate
3470-49-3 4091-26-3, Styrylsulfonyl chloride 5395-71-1, 2-Ethoxyphenyl
isocyanate 5417-63-0, 3-Amino-2-hydroxynaphthalene 6272-38-4,
2-Benzyloxyphenol 6344-59-8, 1-Hydroxy-2-nitrofluorene 13020-57-0,
3-Hydroxybenzophenone 16629-19-9, 2-Thiophenesulfonyl chloride
16744-98-2, 2-Fluorophenyl isocyanate 17337-13-2, 2-Phenylphenyl
isocyanate 17573-92-1, 3-Methoxythiophene 17802-02-7,
3-Chloro-2-nitrophenol 18493-15-7 18704-37-5, 8-Quinolinesulfonyl
chloride 18908-07-1, 3-Methoxyphenyl isocyanate 20513-43-3
21286-54-4 23095-31-0, 3,4-Dimethoxyphenylsulfonyl chloride
23138-55-8, 3-Bromophenyl isocyanate 24615-22-3 35821-29-5
39234-86-1 39262-22-1 40398-01-4, 2-Chloro-6-methylphenyl isocyanate
40411-25-4, 2-Ethylphenyl isocyanate 41195-90-8, 2,3-Dichlorophenyl
isocyanate 52260-30-7, 2-Methylthiophenyl isocyanate 55076-90-9,
2,4-Dibromophenyl isocyanate 63435-16-5, Methyl 4-amino-3-
hydroxybenzoate 65295-69-4, 2,6-Difluorophenyl isocyanate 69812-29-9,
2-Acetamido-4-methyl-5-thiazolesulfonyl chloride 82419-26-9,
2,3-Difluoro-6-nitrophenol 99968-81-7, 3-Iodo-2-hydroxyaniline
126714-85-0, 2,3-Dichlorothiophene-5-sulfonyl chloride 146224-62-6,
5-Aminocarbonyl-2-aminophenol 182500-26-1, 2-Trifluoromethoxyphenyl
isocyanate 182500-27-2, 2-Amino-5,6-diphenylphenol 182500-29-4
182500-30-7, 3,5,6-Trifluoro-2-hydroxyaniline 182500-31-8,
4-Trifluoromethyl-3-fluoro-2-hydroxyaniline 183513-64-6 201532-49-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenylureas as IL-8 receptor antagonists)

IT *87-17-2*, 2-Phenylaminocarbonylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenylureas as IL-8 receptor antagonists)

RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 23 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:113712 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 130:168662
TITLE: Preparation of N-sulfonylproline dipeptide derivatives and analogs as inhibitors of leukocyte adhesion mediated by VLA-4
INVENTOR(S): Thorsett, Eugene D.; Semko, Christopher M.; Pleiss, Michael A.; Kreft, Anthony; Konradi, Andrei W.; Grant, Francine S.; Baudy, Reinhardt Bernhard; Sarantakis, Dimitrios
PATENT ASSIGNEE(S): Athena Neurosciences, Inc., USA; American Home Products Corporation
SOURCE: PCT Int. Appl., 294 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9906437	A1	19990211	WO 1998-US16070	19980731 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2290748	AA	19990211	CA 1998-2290748	19980731 <--
AU 9888234	A1	19990222	AU 1998-88234	19980731 <--
EP 994896	A1	20000426	EP 1998-939871	19980731 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 9811594	A	20000905	BR 1998-11594	19980731 <--
JP 2001512139	T2	20010821	JP 2000-505192	19980731 <--
NO 2000000452	A	20000327	NO 2000-452	20000128 <--
PRIORITY APPLN. INFO.:			US 1997-904423 A2	19970731 <--
			WO 1998-US16070 W	19980731 <--

OTHER SOURCE(S): MARPAT 130:168662
AB Disclosed are title compds. R1SO2NR2CHR3QCHR5COR6 [R1 = (un)substituted alkyl, (un)substituted aryl, (un)substituted cycloalkyl, (un)substituted

heterocyclyl; R2 = H, any group R1; R1R2 may form (un)substituted heterocyclic ring; R3 = H, any group R1; R2R3 may form (un)substituted heterocyclic ring; R5 = CH2X1; X1 = H, OH, acylamino, (un)substituted alkyl, alkoxy, aryloxy, aryl, aryloxyaryl, CO2H, carboxyalkyl, carboxyaryl, carboxyheteroaryl, (un)substituted cycloalkyl, (un)substituted heterocyclyl; Q = C(X)NR7; R7 = H, alkyl; X = O, S; R6 = NH2, (un)substituted alkoxy, (un)substituted cycloalkoxy, succinimidyloxy, adamantylamino, β-cholest-5-en-3-yloxy, NHOY, NH(CH2)pCO2Y, OCH2NR9R10; Y = H, (un)substituted alkyl, (un)substituted aryl; p = 1-8; R9 = (un)substituted CO-aryl; R10 = H, CH2CO2R11, NHSO2Z'; R11 = alkyl; Z' = (un)substituted alkyl, (un)substituted cycloalkyl, (un)substituted aryl, (un)substituted heteroaryl, (un)substituted heterocyclyl; and pharmaceutically acceptable salts thereof, with provisos] which bind VLA-4 (also referred to as integrin α4β1 and CD49d/CD29). Certain of these compds. also inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated by VLA-4. Such compds. are useful in the treatment of inflammatory diseases in a mammalian patient, e.g., human, wherein the disease may be, for example, ***asthma***, Alzheimer's disease, atherosclerosis, ***AIDS*** dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, ***tumor*** metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis. Thus, BOP-mediated peptide coupling of Ts-Pro-OH (Ts = tosyl) with H-Tyr-OMe gave 75% of the corresponding ester, which underwent saponification in quant. yield to give desired dipeptide Ts-Pro-Tyr-OH. All prepared compds. have IC50 ≤ 15 μM in a VLA-4 binding assay.

IC ICM C07K005-078
ICS A61K038-05

CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 15, 63

IT ***AIDS (disease)***
(***AIDS*** dementia complex; preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

IT Mental disorder
(***AIDS*** dementia; preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

IT Anti-Alzheimer's agents
Antiasthmatics
Antidiabetic agents
Antirheumatic agents
Encephalitis
Meningitis
Psoriasis
Transplant and Transplantation
(preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

IT 220149-83-7P 220302-57-8P 220302-58-9P 220302-61-4P 220302-67-0P
220302-69-2P 220302-72-7P 220302-77-2P 220302-80-7P 220302-82-9P
220302-85-2P 220302-86-3P ***220302-91-0P*** 220302-93-2P
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220303-48-0P 220337-23-5P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

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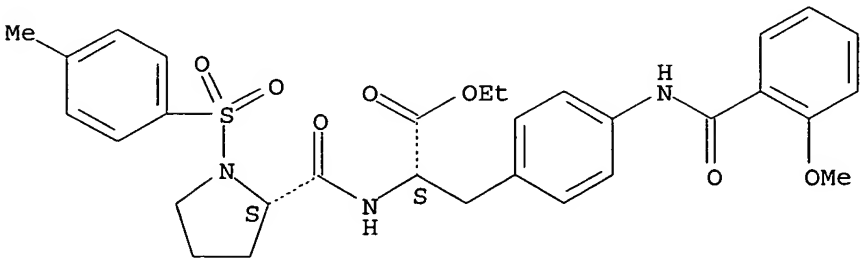
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

IT ***220302-91-0P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

RN 220302-91-0 HCAPLUS

CN L-Phenylalanine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-4-[(2-methoxybenzoyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

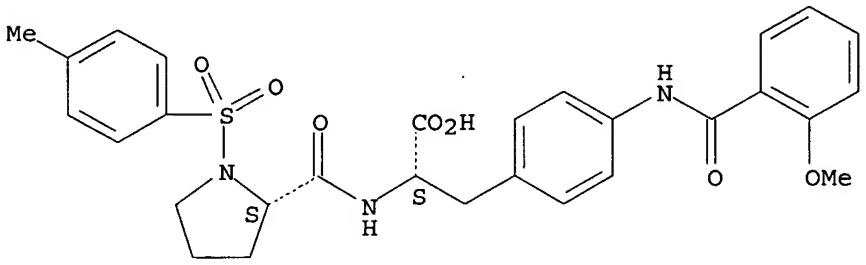


IT ***220302-95-4P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU***

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-sulfonylproline dipeptide derivs. and analogs as inhibitors of leukocyte adhesion mediated by VLA-4)

RN 220302-95-4 HCAPLUS
CN L-Phenylalanine, 1-[(4-methylphenyl)sulfonyl]-L-prolyl-4-[(2-methoxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



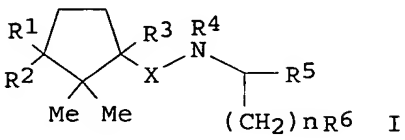
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 24 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:27805 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 130:95843
TITLE: Preparation of cyclopentylcarbonylamino acid as inhibitors of α4β1 mediated cell adhesion
INVENTOR(S): Lobl, Thomas J.; Rishton, Gil; Teegarden, Bradley; Polinsky, Alex; Yamagishi, Masafumi; Tanis, Steven P.; Fisher, Jed F.; Thomas, Edward W.; Chrusciel, Robert A.
PATENT ASSIGNEE(S): Tanabe Seiyaku Co., Ltd., Japan; Pharmacia & Upjohn Company
SOURCE: PCT Int. Appl., 342 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9858902	A1	19981230	WO 1998-US13064	19980623 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9881633	A1	19990104	AU 1998-81633	19980623 <--
EP 991619	A1	20000412	EP 1998-931521	19980623 <--
EP 991619	B1	20030910		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				

JP 2001517246	T2	20011002	JP 1999-504997		19980623 <--
US 6482849	B1	20021119	US 1998-102584		19980623 <--
AT 249421	E	20030915	AT 1998-931521		19980623 <--
PT 991619	T	20040227	PT 1998-931521		19980623 <--
ES 2206953	T3	20040516	ES 1998-931521		19980623 <--
US 2003130349	A1	20030710	US 2002-193137		20020712 <--
US 6596752	B1	20030722			
PRIORITY APPLN. INFO.:			US 1997-50515P	P	19970623 <--
			US 1998-102584	A3	19980623 <--
			WO 1998-US13064	W	19980623 <--

OTHER SOURCE(S): MARPAT 130:95843
GI



I

AB Title compds. [I; n = 0, 1; R1 = H, CH3; R2 = CN, CO2H, CONH2, CONHOCH2Ph, NHCOOCH2Ph, etc.; R3 = H, CH3; X = CH, CO; R4 = H, alkyl; R5 = CO2H, CONH2, COOR, etc.; R = alkyl; R6 = aryl, heteroaryl, arylcarbonyl, aarylcarbonylaminoalkyl, etc.], a pharmaceutically acceptable salt, a stereoisomer thereof are prepared as inhibitors of α4β1 mediated adhesion to either VCAM or CS-1 and which can be used for treating or preventing α4β1 adhesion mediated conditions in human such as inflammatory diseases. Thus, (1S-cis)- N-[(3-carboxy-2,2,3-trimethylcyclopentyl)carbonyl]-O-(phenylmethyl)-L-tyrosine was prepared and assayed for inhibition of β1-mediated cell adhesion in vitro.

IC ICM C07C233-63
ICS C07C233-87; A61K031-16

CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1

IT Allergy
Asthma
Atherosclerosis
Cell adhesion
Eczema
Psoriasis
Rheumatoid arthritis
(preparation of cyclopentylcarbonylamino acid as inhibitors of α4β1 mediated cell adhesion)

IT 219493-88-6P 219493-89-7P 219493-90-0P 219493-91-1P 219493-92-2P
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219496-31-8P 219496-32-9P

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopentylcarbonylamino acid as inhibitors of α4β1 mediated cell adhesion)

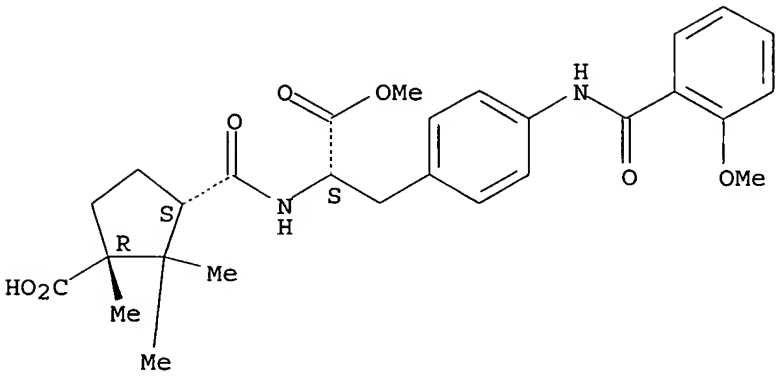
IT ***219494-81-2P 219494-82-3P 219495-16-6P 219495-30-4P***

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of cyclopentylcarbonylamino acid as inhibitors of α4β1 mediated cell adhesion)

RN 219494-81-2 HCAPLUS

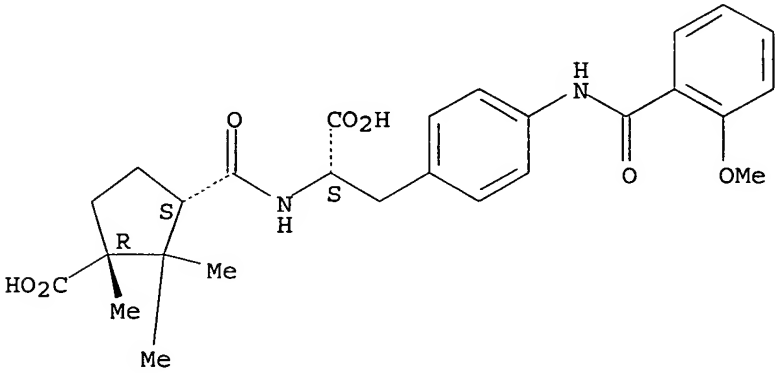
CN L-Phenylalanine, N-[[(1S,3R)-3-carboxy-2,2,3-trimethylcyclopentyl]carbonyl]-4-[(2-methoxybenzoyl)amino]-, α-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



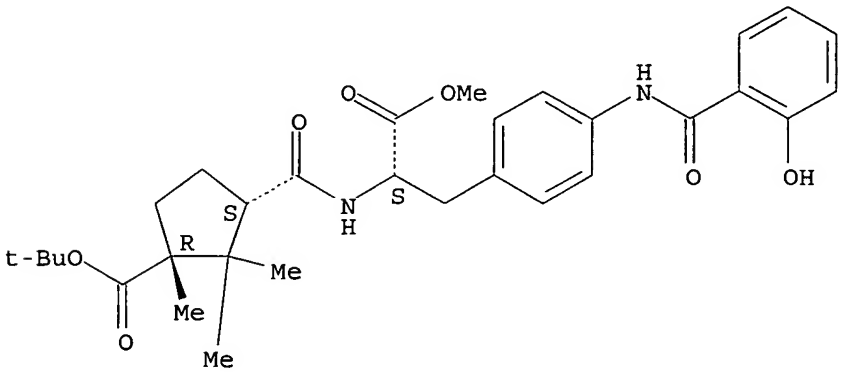
RN 219494-82-3 HCAPLUS
CN L-Phenylalanine, N-[[(1S,3R)-3-carboxy-2,2,3-trimethylcyclopentyl]carbonyl]-4-[(2-methoxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



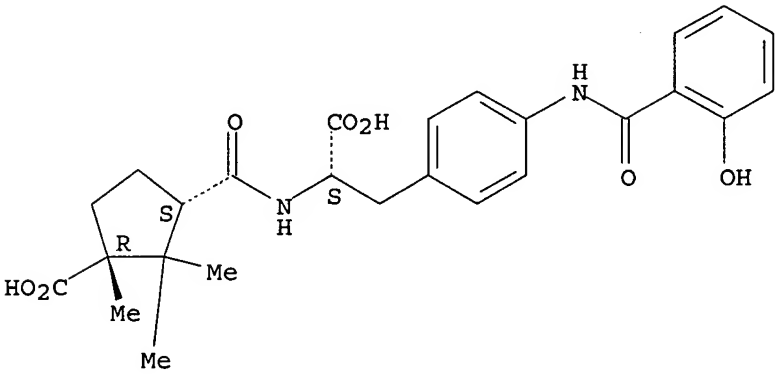
RN 219495-16-6 HCAPLUS
CN L-Phenylalanine, N-[[(1S,3R)-3-[(1,1-dimethylethoxy)carbonyl]-2,2,3-trimethylcyclopentyl]carbonyl]-4-[(2-hydroxybenzoyl)amino]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 219495-30-4 HCAPLUS
CN L-Phenylalanine, N-[[(1S,3R)-3-carboxy-2,2,3-trimethylcyclopentyl]carbonyl]-4-[(2-hydroxybenzoyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 25 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:479029 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 129:122458
TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists
INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Hertzberg, Robert Philip; Rutledge, Melvin Clarence, Jr.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 50 pp., Cont.-in-part of U.S. Ser. No. 641,990.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
US 5780483	A	19980714	US 1996-701299		19960821	<--
US 5886044	A	19990323	US 1996-641990		19960320	<--
US 6211373	B1	20010403	US 1998-111663		19980708	<--
PRIORITY APPLN. INFO.:			US 1995-390260	B2	19950217	<--
			US 1996-641990	A2	19960320	<--
			WO 1996-US2260	W	19960216	<--
			US 1996-701299	A3	19960821	<--

OTHER SOURCE(S): MARPAT 129:122458
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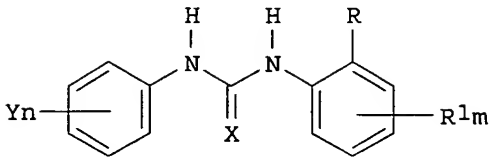


I

AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of ≤10 (sic); R1, Y = H, halo, NO2, cyano, (halo)alkyl, alkenyl, (halo)alkoxy, N3, HO, hydroxyalkyl, aryl, arylalkyl, aryloxy, arylalkoxy, heteroaryl, heteroarylalkyl, heterocyclyl, heterocyclylalkyl, heterocyclylalkoxy, arylalkenyl, heteroarylalkenyl, (un)substituted NH2, CONH2, or SO3H, etc.; m, n = 1-3], which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared Thus, Me 4-amino-3-hydroxybenzoate was added to a solution of Ph isocyanate in PhMe and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4-(methoxycarbonyl)phenyl]-N'-phenylurea.

IC ICM A61K031-47
ICS A61K031-425; A61K031-38; A61K031-17

INCL 514311000

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

ST phenylurea prepn interleukin 8 receptor antagonist; psoriasis treatment diphenylurea prepn; atopic dermatitis treatment diphenylurea; ***asthma*** treatment diphenylurea; chronic obstructive pulmonary disease treatment diphenylurea; adult respiratory distress syndrome treatment diphenylurea; arthritis treatment diphenylurea; inflammatory bowel disease treatment diphenylurea; Crohn disease treatment diphenylurea; ulcerative colitis treatment diphenylurea; septic shock treatment diphenylurea; endotoxic shock treatment diphenylurea; gram neg sepsis treatment diphenylurea; toxic shock syndrome treatment diphenylurea; cardiac renal reperfusion injury treatment diphenylurea; glomeruli nephritis treatment diphenylurea; thrombosis treatment diphenylurea; Alzheimer disease treatment diphenylurea; graft vs host reaction treatment diphenylurea; allograft rejection treatment diphenylurea; stroke treatment diphenylurea

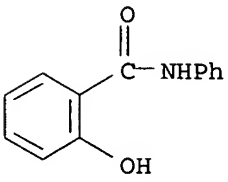
IT 86-84-0, 1-Naphthyl isocyanate ***87-17-2***, 2-Phenylaminocarbonylphenol 88-67-5, 2-Iodobenzoic acid 90-43-7, 2-Phenylphenol 91-93-0 95-54-5, o-Phenylenediamine, reactions 95-55-6, 2-Aminophenol 98-09-9, Phenylsulfonyl chloride 98-17-9, α,α,α-Trifluoro-m-cresol 99-56-9, 4-Nitro-1,2-phenylenediamine 99-57-0, 5-Nitro-2-hydroxyaniline 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 106-40-1, 4-Bromoaniline 116-63-2 117-77-1, 2-Hydroxy-3-aminoanthraquinone 117-99-7 121-51-7, 3-Nitrobenzenesulfonyl chloride 121-60-8, 4-Acetamidophenylsulfonyl chloride 121-88-0, 2-Amino-5-nitrophenol 124-38-9, Carbon dioxide, reactions 137-07-5, 2-Aminothiophenol 274-09-9, 1,3-Benzodioxole 320-76-3 329-01-1, 3-Trifluoromethylphenyl isocyanate 385-01-3, 2-Nitro-3-fluorophenol 394-31-0, 2-Amino-5-hydroxybenzoic acid 394-33-2, 4-Fluoro-2-nitrophenol 400-98-6, 4-Amino-3-nitrobenzotrifluoride 444-30-4, 2-Trifluoromethylphenol 446-36-6, 5-Fluoro-2-nitrophenol 463-71-8, Thiophosgene 534-85-0, 2-Hydroxy-3-aminobenzoic acid 544-92-3, Copper(I) cyanide 570-23-0, 2-Anilinoaliline 576-24-9, 2,3-Dichlorophenol 580-51-8, 3-Phenylphenol 603-87-2,

2-Hydroxy-3-nitroaniline 609-89-2, 4,6-Dichloro-2-nitrophenol 611-20-1, 2-Cyanophenol 614-68-6, 2-Methylphenyl isocyanate 615-36-1, 2-Bromoaniline 618-45-1, 3-Isopropylphenol 620-17-7, 3-Ethylphenol 644-35-9, 2-Propylphenol 700-87-8, 2-Methoxyphenyl isocyanate 776-04-5, 2-(Trifluoromethyl)benzenesulfonyl chloride 837-95-6, 2-Nitro-4-(trifluoromethyl)benzenesulfonyl chloride 873-62-1, 3-Cyanophenol 1548-13-6, 4-Trifluoromethylphenyl isocyanate 1592-00-3, 2-Bromophenyl isocyanate 1623-92-3, 4-Phenoxyphenylsulfonyl chloride 1762-95-4 1899-93-0, 3-Methylbenzenesulfonyl chloride 1939-99-7, Benzylsulfonyl chloride 2237-30-1, 3-Cyanoaniline 2243-42-7, 2-Phenoxybenzoic acid 2285-12-3, 2-Trifluoromethylphenyl isocyanate 2374-03-0, 3-Hydroxy-4-aminobenzoic acid 2493-02-9, 4-Bromophenyl isocyanate 2612-57-9, 2,4-Dichlorophenyl isocyanate 2834-92-6, 1-Amino-2-hydroxynaphthalene 2835-98-5, 2-Hydroxy-4-methylaniline 3272-08-0, 2-Nitro-4-cyanophenol 3320-83-0, 2-Chlorophenyl isocyanate 3320-86-3, 2-Nitrophenyl isocyanate 3470-49-3, 5-Hydroxy-1-indanone 4091-26-3, Styrylsulfonyl chloride 5395-71-1, 2-Ethoxyphenyl isocyanate 5417-63-0, 3-Amino-2-hydroxynaphthalene 6344-59-8, 1-Hydroxy-2-nitrofluorene 7664-41-7, Ammonia, reactions 13020-57-0, 3-Hydroxybenzophenone 13360-57-1, Dimethylsulfamoyl chloride 14755-02-3 16629-19-9, 2-Thiophenesulfonyl chloride 16744-98-2, 2-Fluorophenyl isocyanate 17337-13-2, 2-Phenylphenyl isocyanate 17573-92-1, 3-Methoxythiophene 17802-02-7, 3-Chloro-2-nitrophenol 18162-48-6, Tert-Butyldimethylsilyl chloride 18493-15-7 18704-37-5, 8-Quinolinesulfonyl chloride 18908-07-1, 3-Methoxyphenyl isocyanate 20513-43-3 21286-54-4, (+)-10-Camphorsulfonyl chloride 23095-31-0, 3,4-Dimethoxyphenylsulfonyl chloride 24615-22-3 26386-88-9, Diphenylphosphoryl azide 26628-22-8, Sodium azide 32315-10-9, Triphosgene 35821-29-5 39234-86-1 39262-22-1, (-)-10-Camphorsulfonyl chloride 40398-01-4, 2-Chloro-6-methylphenyl isocyanate 40411-25-4, 2-Ethylphenyl isocyanate 41195-90-8, 2,3-Dichlorophenyl isocyanate 43115-40-8, 2-Amino-4-(ethylsulfonyl)phenol 52260-30-7, 2-Methylthiophenyl isocyanate 55076-90-9, 2,4-Dibromophenyl isocyanate 63435-16-5, Methyl 4-amino-3-hydroxybenzoate 65295-69-4, 2,6-Difluorophenyl isocyanate 69812-29-9, 2-Acetamido-4-methyl-5-thiazolesulfonyl chloride 82419-26-9, 2,3-Difluoro-6-nitrophenol 93254-81-0, 2-Benzyloxybenzophenone 99968-81-7, 3-Iodo-2-hydroxyaniline 126714-85-0, 2,3-Dichlorothiophene-5-sulfonyl chloride 146224-62-6, 5-Aminocarbonyl-2-aminophenol 182500-26-1, 2-Trifluoromethoxyphenyl isocyanate 182500-27-2, 2-Amino-5,6-diphenylphenol 182500-28-3, 2-Nitro-5-methyl-4-bromophenol 182500-29-4 182500-30-7, 3,5,6-Trifluoro-2-hydroxyaniline 182500-31-8, 4-Trifluoromethyl-3-fluoro-2-hydroxyaniline 183513-64-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

IT ***87-17-2***, 2-Phenylaminocarbonylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

RN 87-17-2 HCAPLUS

CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 26 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:268489 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 128:321568
TITLE: Anthranilic acid derivatives as multi drug resistance modulators
INVENTOR(S): Ryder, Hamish; Ashworth, Philip Anthony; Roe, Michael John; Brumwell, Julie Elizabeth; Hunjan, Sukhjit; Folkes, Adrian John; Sanderson, Jason Terry; Williams, Susannah; Maximen, Levi Michael; et al.
PATENT ASSIGNEE(S): Xenova Ltd., UK; Ryder, Hamish; Ashworth, Philip Anthony; Roe, Michael John; Brumwell, Julie Elizabeth; Hunjan, Sukhjit; Folkes, Adrian John; Sanderson, Jason Terry; Williams, Susannah; Maximen, Levi Michael
SOURCE: PCT Int. Appl., 203 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9817648	A1	19980430	WO 1997-GB2885	19971017 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
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AU 9746339	A1	19980515	AU 1997-46339	19971017 <--
AU 741922	B2	20011213		
ZA 9709329	A	19990419	ZA 1997-9329	19971017 <--
EP 934276	A1	19990811	EP 1997-945030	19971017 <--
EP 934276	B1	20031217		
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BR 9711935	A	19990824	BR 1997-11935	19971017 <--
GB 2334521	A1	19990825	GB 1999-8193	19971017 <--
GB 2334521	B2	20001004		
CN 1241181	A	20000112	CN 1997-180708	19971017 <--
JP 2001502683	T2	20010227	JP 1998-519108	19971017 <--
RU 2195454	C2	20021227	RU 1999-109990	19971017 <--
AT 256663	E	20040115	AT 1997-945030	19971017 <--
PT 934276	T	20040531	PT 1997-945030	19971017 <--

ES 2210586	T3	20040701	ES 1997-945030		19971017 <--
SK 284649	B6	20050804	SK 1999-509		19971017 <--
PL 191150	B1	20060331	PL 1997-332725		19971017 <--
TW 498074	B	20020811	TW 1997-86115402		19971018 <--
BG 103327	A	20001130	BG 1999-103327		19990413 <--
NO 9901836	A	19990617	NO 1999-1836		19990416 <--
NO 313591	B1	20021028			
KR 2000049278	A	20000725	KR 1999-703389		19990417 <--
US 6218393	B1	20010417	US 1999-284642		19990609 <--
HK 1019330	A1	20010112	HK 1999-103773		19990901 <--
PRIORITY APPLN. INFO.:			WO 1996-GB2552	A	19961018 <--
			GB 1997-17576	A	19970819 <--
			WO 1997-GB2885	W	19971017 <--

OTHER SOURCE(S): MARPAT 128:321568
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Anthranilic acid derivs. I [R, R1, R2 = H, alkyl, OH, alkoxy, halo, NO2, amino; or R1R2 = OCH2O or OCH2CH2O; R3 = H, alkyl; R4 = alkyl, or CH2 or CH2CH2 bridged to either Ph ring; R5 = H, OH, alkyl; X = bond, O, S, S(CH2)p, O(CH2)p; p = 1-6; R6 = H, alkyl, alkoxy; q = 0 or 1; Ar = (un)saturated carbo- or heterocyclic; R7, R8 = H, (un)substituted alkyl, alkoxy, OH, halo, Ph, NHOH, NO2, amino, SH, alkylthio; or R7R8 = CH:CHCH:CH or OCH2O; n = 0, 1; m = 0-6] and their pharmaceutically acceptable salts are disclosed. The compds. are inhibitors of P-glycoprotein, and may thus be used, inter alia, as modulators of multidrug resistance in the treatment of multidrug-resistant ***cancers***, for example, to potentiate the cytotoxicity of a ***cancer*** drug. For instance, amidation of 3-quinolinecarboxylic acid with the corresponding aminothiophene derivative via the acid chloride gave title compound II in 44% yield. In a test for potentiation of doxorubicin toxicity to AR 1.0 cells, II had a potentiation index of 142 at 30 nM.

IC ICM C07D217-04
ICS A61K031-47

CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 25

IT

206872-32-4P	206872-33-5P	206872-34-6P	206872-35-7P	206872-36-8P
206872-38-0P	206872-39-1P	206872-40-4P	206872-41-5P	206872-42-6P
206872-43-7P	206872-44-8P	206872-45-9P	206872-46-0P	206872-47-1P
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206874-21-7P 206874-22-8P 206874-23-9P 206874-24-0P 206874-25-1P
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206874-33-1P

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilic acid derivs. as multi-drug resistance modulators)

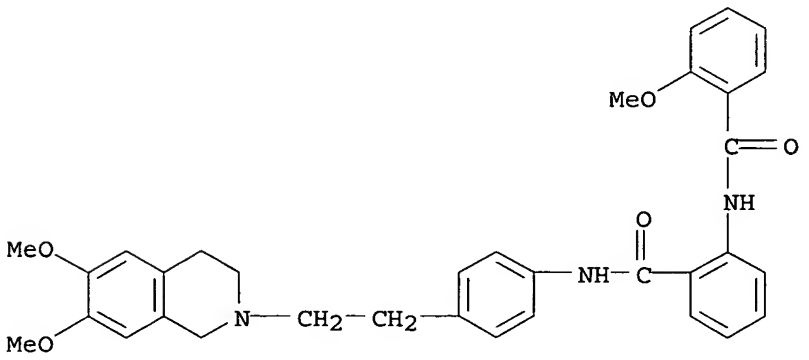
IT ***206874-03-5P 206874-06-8P 206874-09-1P***

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilic acid derivs. as multi-drug resistance modulators)

RN 206874-03-5 HCAPLUS

CN Benzamide, N-[2-[[[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]amino]carbonyl]phenyl]-2-methoxy- (9CI) (CA INDEX NAME)



RN 206874-06-8 HCAPLUS

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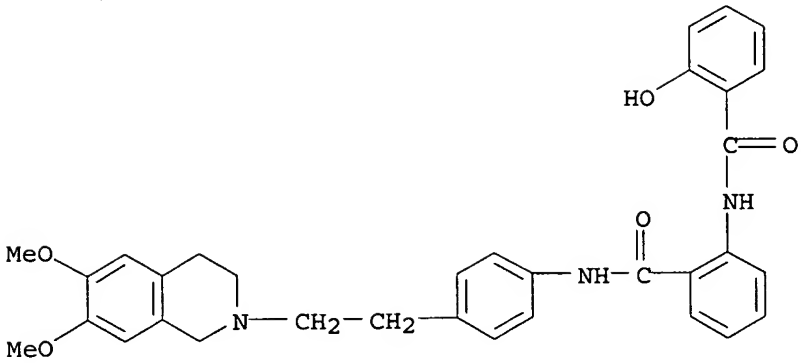
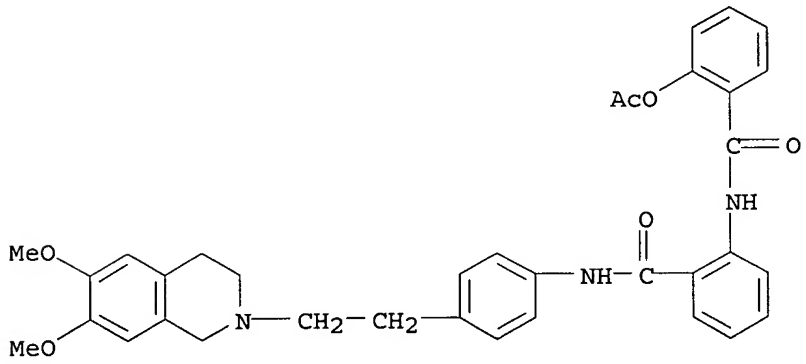


RN 206874-09-1 HCAPLUS
CN Benzamide, 2-[[2-(acetyloxy)benzoyl]amino]-N-[4-[2-(3,4-dihydro-6,7-dimethoxy-2(1H)-isoquinolinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

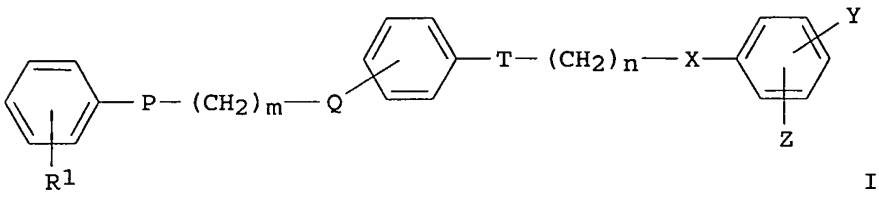


REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L101 ANSWER 27 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:672686 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 127:262527
TITLE: Leukotriene antagonistic benzoic acid derivatives
INVENTOR(S): Abram, Trevor Smyth; Cuthbert, Nigel James; Francis, Hilary Patricia; Gardiner, Phillip John; Norman, Peter; Tudhope, Stephen Richard
PATENT ASSIGNEE(S): Bayer A.-G., Germany
SOURCE: Can. Pat. Appl., 76 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2190801	AA	19970524	CA 1996-2190801	19961120 <--

EP 791576 A2 19970827 EP 1996-118040 19961111 <--
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
US 5872280 A 19990216 US 1996-748331 19961113 <--
JP 09169712 A2 19970630 JP 1996-325841 19961122 <--
PRIORITY APPLN. INFO.: GB 1995-23946 A 19951123 <--
OTHER SOURCE(S): MARPAT 127:262527
GI



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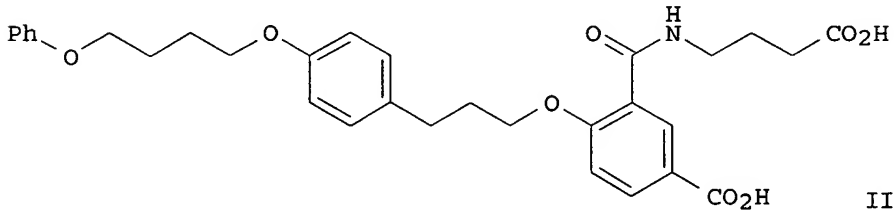

II

AB The invention relates to benzoic acid derivs. I [R1 = H, alkyl, substituted Ph; P, Q = O, S, bond; X = O, S, CONH; T = CH2CH2, O, S, bond; Y = CO2H, NHSO2R3, CONHSO2R3; R2 = H, halo, CF3, CF3O, NO2, cyano, alkyl, or alkoxy; Z = CO2H, COR4, CO(CH2)pCO2H, O(CH2)pCO2H, S(CH2)pCO2H, NO2, CONHWCO2H, NHWCO2H; R3 = CF3, alkyl, (un)substituted Ph; R4 = WCO2H, alkyl; p = 0-5; W = phenylene or alkylene optionally substituted by alkyl or cycloalkyl, CO(CH2)q, (CH2)q; q = 0-5; m = 0-6; n = 0-4] and their salts. The compds. are leukotriene antagonists, and therefore are suitable as active ingredients in medicaments, particularly for the treatment of respiratory diseases such as ***asthma***. For instance, amidation of H2N(CH2)3CO2Me with Me 4-hydroxyisophthalate, followed by etherification of the phenolic OH with 4-[PhO(CH2)4O]C6H4(CH2)3I using K2CO3 in DMF, and saponification using LiOH in aqueous THF, gave a preferred title compound, II. In assays for inhibition of LTD4- and LTC4-induced contraction of guinea-pig trachea, II had pKB values of 6.9 and 7.2, resp.

IC ICM C07C236-74
ICS C07C236-38; C07C236-64; C07C206-69; C07C323-40; C07C311-08; C07C311-21; A61K031-19; A61K031-276
CC 25-17 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1
ST benzoic acid prepn leukotriene antagonist; ***antiasthmatic*** antiinflammatory benzoic acid prepn
IT Anti-inflammatory agents
Antiasthmatics
(preparation of benzoic acid derivs. as leukotriene antagonists)
IT 196103-06-7P 196103-07-8P 196103-08-9P ***196103-09-0P***

196103-10-3P 196103-11-4P 196103-12-5P 196103-13-6P
196103-14-7P 196103-15-8P 196103-16-9P 196103-17-0P 196103-18-1P
196103-19-2P 196103-20-5P 196103-21-6P 196103-22-7P 196103-23-8P
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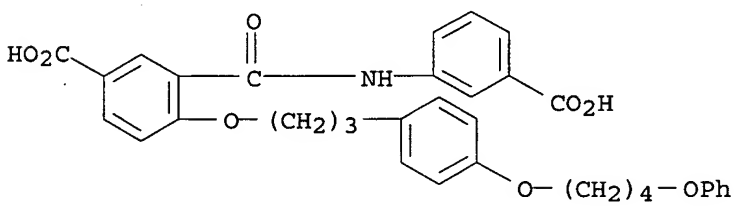
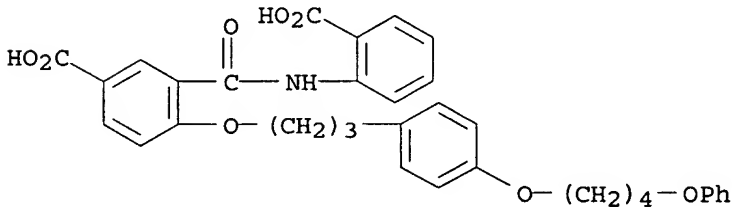
196103-30-7P 196103-31-8P 196103-32-9P 196103-33-0P 196103-34-1P
196103-35-2P 196103-36-3P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid derivs. as leukotriene antagonists)

IT ***196103-09-0P 196103-10-3P 196103-11-4P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzoic acid derivs. as leukotriene antagonists)

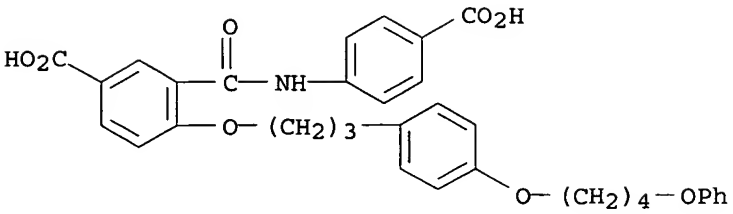
RN 196103-09-0 HCAPLUS
CN Benzoic acid, 3-[[(3-carboxyphenyl)amino]carbonyl]-4-[3-[4-(4-phenoxybutoxy)phenyl]propoxy]- (9CI) (CA INDEX NAME)



RN 196103-10-3 HCAPLUS
CN Benzoic acid, 3-[[(2-carboxyphenyl)amino]carbonyl]-4-[3-[4-(4-phenoxybutoxy)phenyl]propoxy]- (9CI) (CA INDEX NAME)



RN 196103-11-4 HCAPLUS
CN Benzoic acid, 3-[[(4-carboxyphenyl)amino]carbonyl]-4-[3-[4-(4-phenoxybutoxy)phenyl]propoxy]- (9CI) (CA INDEX NAME)

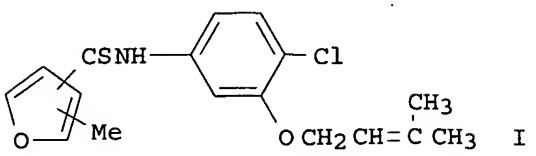


L101 ANSWER 28 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:479342 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 127:95191
TITLE: Preparation of furan- and thiophenecarbothioamide derivatives and their use as inhibitors of the replication of ***HIV***-1 and ***HIV***-1 mutants
INVENTOR(S): Brouwer, Walter Gerhard; Osika, Ewa Maria; Pierce, Benjamin James
PATENT ASSIGNEE(S): Uniroyal Chemical Company, Inc., USA; Uniroyal Chemical Ltd./uniroyal Chemical Ltee
SOURCE: PCT Int. Appl., 35 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9719940	A1	19970605	WO 1996-US18394	19961115 <--
W: AU, BR, CA, CN, HU, JP, KR, MX, NZ				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5696151	A	19971209	US 1995-565493	19951130 <--
TW 448169	B	20010801	TW 1996-85113662	19961108 <--
ZA 9609490	A	19970602	ZA 1996-9490	19961112 <--
CA 2237194	AA	19970605	CA 1996-2237194	19961115 <--
CA 2237194	C	20060613		
AU 9711199	A1	19970619	AU 1997-11199	19961115 <--
AU 704086	B2	19990415		
EP 874839	A1	19981104	EP 1996-942010	19961115 <--
EP 874839	B1	20020918		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1203596	A	19981230	CN 1996-198705	19961115 <--
CN 1098847	B	20030115		
BR 9611838	A	19990309	BR 1996-11838	19961115 <--
JP 11504657	T2	19990427	JP 1997-520533	19961115 <--
JP 3027771	B2	20000404		
AP 902	A	20001123	AP 1998-1245	19961115 <--
W: GM, GH, KE, LS, MW, SD, SZ, UG, ZW				
AT 224382	E	20021015	AT 1996-942010	19961115 <--
PT 874839	T	20030228	PT 1996-942010	19961115 <--
ES 2183986	T3	20030401	ES 1996-942010	19961115 <--
HK 1016601	A1	20030905	HK 1999-101720	19990421 <--

PRIORITY APPLN. INFO.: US 1995-565493 A 19951130 <--
WO 1996-US18394 W 19961115 <--

OTHER SOURCE(S): MARPAT 127:95191
GI



I

AB Compds. of formula (I), wherein X = O or S. The compds. of this invention are useful for the inhibition of the replication of human immunodeficiency virus-1 (***HIV***-1) and reverse transcriptase (RT) mutants thereof, in vitro and in vivo. The compds. are useful in the therapeutic or prophylactic treatment of diseases caused by ***HIV***-1 and RT mutants thereof, such as acquired immune deficiency syndrome (***AIDS***). Thus, N-[4-chloro-3-(3-methyl-2-butenyloxy)phenyl]-2-methyl-3-furancarboxamide 4, sodium bicarbonate 7.4, and Lawesson's reagent 3.6g were heated to 85°C and held at 85° for 2.5 h to give 2.6g of I (X = O). I (X = O) showed EC50 syncytium formation inhibiting values of 0.003, 0.006, 0.005, 0.005, 0.011, and 0.50 μg/mL for ***HIV***-1 infected cells 100-Ile, 103-Asn, 106-Ala, 138-Lys, 181-Cys, and 188-Leu, resp.

IC ICM C07D307-68
ICS C07D333-38; A61K031-34; A61K031-38

CC 27-8 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1, 63

ST furancarbothioamide thiophenecarbothioamide prepn; ***HIV1*** replication inhibitor; acquired immune deficiency syndrome; mutant ***HIV1*** replication inhibitor; virucide

IT ***AIDS (disease)***
Antiviral agents
Human immunodeficiency virus 1
(preparation of furan- and thiophenecarbothioamide derivs. used as inhibitors of replication of ***HIV***-1 and ***HIV***-1 mutants)

IT 135812-51-0P 135812-52-1P 135812-68-9P 135813-03-5P 135813-04-6P
135813-05-7P 135813-46-6P 165391-80-0P 165391-82-2P 165391-83-3P
165391-84-4P 172998-56-0P 172998-57-1P 172998-58-2P 172998-60-6P
172998-62-8P 172998-75-3P 172998-76-4P 172998-77-5P 173046-03-2P
173046-05-4P 178869-90-4P 178869-91-5P 178869-92-6P 178869-93-7P
178869-94-8P 178869-95-9P 178869-96-0P 178869-97-1P 178870-03-6P
178870-04-7P 178870-05-8P 178870-06-9P 178870-07-0P 178870-08-1P
178870-09-2P 178870-10-5P 178870-11-6P 178870-12-7P
178870-13-8P 178870-14-9P 178870-15-0P 178870-16-1P 178870-17-2P
178870-18-3P 178870-19-4P 178870-29-6P 178870-31-0P 178870-32-1P
178870-33-2P 178870-34-3P 178870-35-4P 178870-36-5P 178870-37-6P
178870-38-7P 178870-39-8P 178870-40-1P 178870-41-2P 178870-42-3P
178870-43-4P 178870-44-5P 178870-46-7P 178870-47-8P 178870-49-0P
178870-50-3P 178870-51-4P 178870-52-5P 178870-54-7P 178870-55-8P
180034-55-3P 180034-56-4P 191984-40-4P 191984-41-5P 191984-42-6P
191984-43-7P 191984-44-8P 191984-45-9P 191984-46-0P 191984-47-1P
191984-48-2P 191984-49-3P 191984-50-6P 191984-51-7P 191984-52-8P
191984-53-9P 191984-54-0P 191984-55-1P 191984-56-2P 191984-57-3P

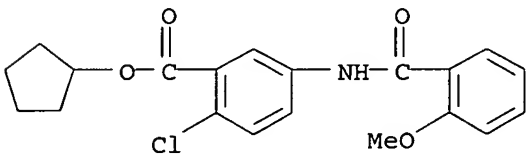
191984-58-4P 191984-59-5P 191984-60-8P 191984-61-9P 191984-62-0P
191984-63-1P 191984-64-2P 191984-65-3P 191984-66-4P 191984-67-5P
191984-68-6P 191984-69-7P 191984-70-0P 191984-71-1P 191984-72-2P
191984-73-3P 191984-74-4P 191984-75-5P 191984-76-6P 191984-77-7P
191984-78-8P 191984-79-9P 191984-80-2P 191984-81-3P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of furan- and thiophenecarbothioamide derivs. used as inhibitors of replication of ***HIV***-1 and ***HIV***-1 mutants)

IT 97-97-2, Chloroacetaldehyde dimethylacetal 121-88-0, 2-Amino-5-nitrophenol 554-14-3, 2-Methylthiophene 870-63-3 7719-09-7, Thionyl chloride 7726-95-6, Bromine, reactions 19172-47-5, Lawesson's reagent
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of furan- and thiophenecarbothioamide derivs. used as inhibitors of replication of ***HIV***-1 and ***HIV***-1 mutants)

IT 619-10-3P, 2-Chloro-5-nitrophenol 5555-00-0P, 2-Methyl-3-furoyl chloride 6947-94-0P, 2-Methyl-3-furancarboxylic acid 29421-73-6P, 3,5-Dibromo-2-methylthiophene 30319-05-2P, 3-Bromo-2-methylthiophene 191984-82-4P 191984-84-6P 191984-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of furan- and thiophenecarbothioamide derivs. used as inhibitors of replication of ***HIV***-1 and ***HIV***-1 mutants)

IT ***178870-09-2P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of furan- and thiophenecarbothioamide derivs. used as inhibitors of replication of ***HIV***-1 and ***HIV***-1 mutants)

RN 178870-09-2 HCAPLUS
CN Benzoic acid, 2-chloro-5-[(2-methoxybenzoyl)amino]-, cyclopentyl ester (9CI) (CA INDEX NAME)



L101 ANSWER 29 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:195707 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 126:186000
TITLE: Novel azepanes and their ring homologs for therapy and prophylaxis of protein kinase mediated diseases
INVENTOR(S): Barbier, Pierre; Stadlwieser, Josef; Taylor, Sven
PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

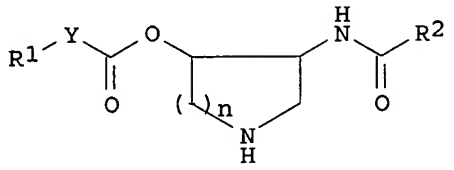
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9702249	A1	19970123	WO 1996-EP2775	19960626 <--
W: AU, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, NZ, PL, RU, SG, TR				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2225616	AA	19970123	CA 1996-2225616	19960626 <--
AU 9663051	A1	19970205	AU 1996-63051	19960626 <--
AU 716996	B2	20000316		
EP 836592	A1	19980422	EP 1996-922032	19960626 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 10510296	T2	19981006	JP 1996-504775	19960626 <--
CN 1199396	A	19981118	CN 1996-195051	19960626 <--
ZA 9605540	A	19970106	ZA 1996-5540	19960628 <--
US 5907038	A	19990525	US 1997-831269	19970331 <--
US 6136969	A	20001024	US 1998-215611	19981217 <--

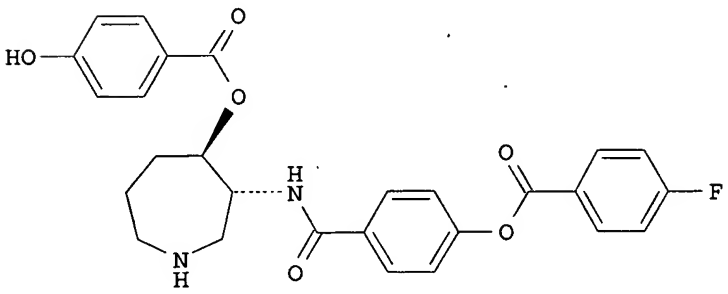
PRIORITY APPLN. INFO.:

EP 1995-110473	A	19950705 <--
US 1996-661276	B1	19960610 <--
WO 1996-EP2775	W	19960626 <--
US 1997-831269	A1	19970331 <--

OTHER SOURCE(S): MARPAT 126:186000
GI



I



II

AB Title compds. I [R1 = Ph or α- or β-naphthyl, all optionally substituted by OH, alkyl, alkoxy, alkoxycarbonyl, PhO, acyloxy, hydroxyphenoxysulfonyl, halo, NO2, amino, acylamino, or N-lower-alkyl-acylamino; R2 = Ph optionally substituted by OH or acyloxy; Y = bond or vinylene; n = 1, 2, or 3] and their pharmaceutically acceptable acid addition salts are protein kinase inhibitors, useful for

treatment of mediated disorders such as inflammation. Over 30 compds. I and many precursors are listed, and the final synthetic steps for 3 compds. I, e.g. II.HCl, are described in detail. Five selected I had IC50 values of 8.8-30 mM for protein kinase C, and 0.041-1.9 mM for protein kinase A. Several I also stimulated DNA synthesis in mouse hair follicles, with EC50 of 5-40 μM.

IC ICM C07D223-12
ICS C07D211-56; C07D207-14; A61K031-55; A61K031-445; A61K031-40

CC 27-21 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1

IT Anti-***AIDS*** agents
Anti-inflammatory agents
Antiarthritics
Antiasthmatics
Anticoagulants
Antitumor agents
Antiviral agents
Bronchodilators
Cardiovascular agents
Immunosuppressants
Platelet aggregation inhibitors
(preparation of azepanes and ring homologs as protein kinase inhibitors)

IT ***Human immunodeficiency virus***
(treatment of infection; preparation of azepanes and ring homologs as protein kinase inhibitors)

IT 187612-72-2P 187612-74-4P 187612-76-6P 187612-78-8P 187612-80-2P
187612-83-5P 187612-86-8P 187612-89-1P 187612-92-6P 187612-95-9P
187612-98-2P 187613-01-0P 187613-04-3P 187613-07-6P 187613-10-1P
187613-14-5P 187613-18-9P 187613-22-5P 187613-26-9P 187613-30-5P
187613-34-9P 187613-38-3P 187613-42-9P ***187613-45-2P***
187613-48-5P 187613-51-0P 187613-54-3P 187613-56-5P 187613-59-8P
187613-62-3P 187613-64-5P 187613-66-7P 187614-29-5P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azepanes and ring homologs as protein kinase inhibitors)

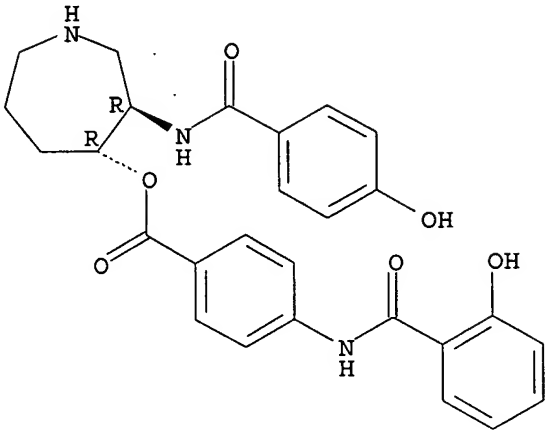
IT ***187613-45-2P***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azepanes and ring homologs as protein kinase inhibitors)

RN 187613-45-2 HCAPLUS
CN Benzoic acid, 4-[(2-hydroxybenzoyl)amino]-, hexahydro-3-[(4-hydroxybenzoyl)amino]-1H-azepin-4-yl ester, (3R-trans)-, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

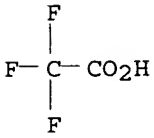
CRN 187613-44-1
CMF C27 H27 N3 O6

Absolute stereochemistry.



CM 2

CRN 76-05-1
CMF C2 H F3 O2



L101 ANSWER 30 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:94060 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 126:104109
TITLE: Tricyclic diazepines useful as GnRH receptor antagonists.
INVENTOR(S): Ohkawa, Shigenori; Fujii, Nobuhiro; Kato, Koichi
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 86 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9638438	A1	19961205	WO 1996-JP1463	19960530 <--

W: AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

CA 2213510	AA	19961205	CA 1996-2213510		19960530 <--
AU 9658448	A1	19961218	AU 1996-58448		19960530 <--
JP 09048777	A2	19970218	JP 1996-137181		19960530 <--
EP 828731	A1	19980318	EP 1996-920006		19960530 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
CN 1217723	A	19990526	CN 1996-194293		19960530 <--
CN 1072219	B	20011003			
US 5866567	A	19990202	US 1996-666430		19960625 <--
PRIORITY APPLN. INFO.:			JP 1995-135376	A	19950601 <--
			WO 1996-JP1463	W	19960530 <--

OTHER SOURCE(S): MARPAT 126:104109
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A = benzene ring; B = 6-membered hydrocarbon ring; X = alkylene, CO, SO; Y = bond, O, NR1; R1 = H or alkyl; R = H, aromatic, alkyl (un)substituted by aromatic; m, n = 1-3] and salts thereof have potent GnRH receptor-antagonizing activity. For example, 2,3,9,10a-tetrahydrobenzo[b]cyclopenta[e][1,4]diazepin-10(1H)-one underwent a sequence of: (1) N9-alkylation by 4-nitrobenzyl bromide (71%); (2) reduction of the tetrahydro system to a hexahydro system with NaBH3CN (70%); (3) hydrogenation of the nitro group (71%); (4) acylation of the resulting amine with PhCH2OCOCl (79%); (5) N4-acylation with BrCH2COBr (66%); and (6) reaction of the bromide with 3,4,5,6-tetrahydrophthalimide (86%), to give title compound II. In an assay for inhibition of 125I-leuprolerin binding to human GnRH receptor in vitro, II had an IC50 of 0.07 μM.

IC ICM C07D403-06
ICS C07D401-14; A61K031-55

CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 2

IT ***Uterus, neoplasm***
Uterus, neoplasm
(myoma, treatment; preparation of tricyclic diazepines useful as GnRH receptor antagonists)

IT Mammary gland
Prostate gland
(***neoplasm***, treatment; preparation of tricyclic diazepines useful as GnRH receptor antagonists)

IT ***Myoma***
Myoma
(uterine, treatment; preparation of tricyclic diazepines useful as GnRH receptor antagonists)

IT 185953-30-4P 185953-32-6P 185953-34-8P 185953-36-0P 185953-38-2P
185953-40-6P 185953-42-8P 185953-44-0P 185953-46-2P 185953-48-4P
185953-49-5P 185953-50-8P ***185953-52-0P*** 185953-54-2P
185953-56-4P 185953-57-5P 185953-58-6P 185953-60-0P 185953-61-1P
185953-62-2P 185953-63-3P 185953-64-4P 185953-66-6P 185953-68-8P
185953-69-9P 185953-70-2P 185953-71-3P 185953-72-4P 185953-73-5P
185953-74-6P 185953-75-7P 185953-77-9P
RL: AGR (Agricultural use); ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tricyclic diazepines useful as GnRH receptor antagonists)

IT ***185953-52-0P***

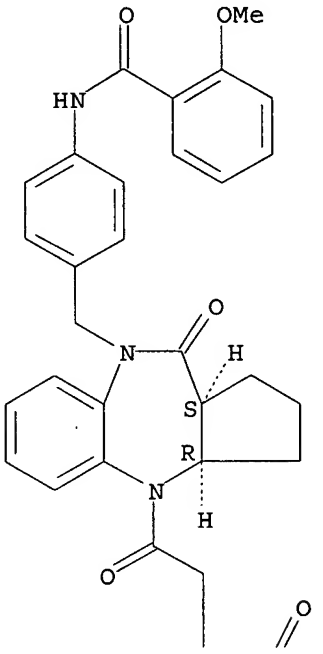
RL: AGR (Agricultural use); ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of tricyclic diazepines useful as GnRH receptor antagonists)

RN 185953-52-0 HCAPLUS

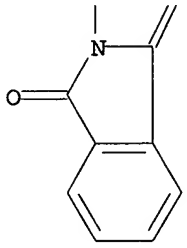
CN Benzamide, N-[4-[[4-[(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)acetyl]-2,3,3a,4,10,10a-hexahydro-10-oxobenzo[b]cyclopenta[e][1,4]diazepin-9(1H)-yl]methyl]phenyl]-2-methoxy-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 2-A



L101 ANSWER 31 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:643902 HCAPLUS <<LOGINID::20061006>>

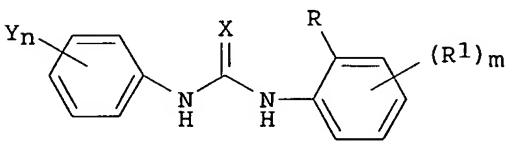
DOCUMENT NUMBER: 125:275430
TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists
INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Rutledge, Melvin Clarence, Jr.; Hertzberg, Robert Philip
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625157	A1	19960822	WO 1996-US2260	19960216 <--
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 809492	A1	19971203	EP 1996-906547	19960216 <--
R: BE, CH, DE, DK, FR, GB, IT, LI, NL				
JP 11503110	T2	19990323	JP 1996-525199	19960216 <--
CA 2432662	AA	19970821	CA 1996-2432662	19960821 <--
WO 9729743	A1	19970821	WO 1996-US13632	19960821 <--
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9669007	A1	19970902	AU 1996-69007	19960821 <--
AU 725456	B2	20001012		
EP 896531	A1	19990217	EP 1996-929723	19960821 <--
R: AT, ES, GR, LU, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1215990	A	19990505	CN 1996-180245	19960821 <--
JP 2000504722	T2	20000418	JP 1997-529318	19960821 <--
NZ 316710	A	20000526	NZ 1996-316710	19960821 <--
BR 9612779	A	20001024	BR 1996-12779	19960821 <--
CN 1539816	A	20041027	CN 2004-10032423	19960821 <--
US 6005008	A	19991221	US 1997-894291	19970815 <--
US 6211373	B1	20010403	US 1998-111663	19980708 <--
NO 9803737	A	19981014	NO 1998-3737	19980814 <--
US 6180675	B1	20010130	US 1999-240354	19990129 <--

PRIORITY APPLN. INFO.:

US 1995-390260	A2	19950217 <--
WO 1996-US2260	W	19960216 <--
US 1996-641990	A3	19960320 <--
CA 1996-2245927	A3	19960821 <--
US 1996-701299	A3	19960821 <--
WO 1996-US13632	W	19960821 <--

OTHER SOURCE(S): MARPAT 125:275430
GI



I

AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of ≤10; R1, Y = H, halo, NO2, cyano, C1-10 (halo)alkyl, C2-10 alkenyl, C1-10 (halo)alkoxy, N3, HO, C1-4 hydroxyalkyl, aryl, aryl-C1-4 alkyl, aryloxy, aryl-C1-4 alkoxy, heteroaryl, heteroarylalkyl, heterocyclyl, heterocyclyl-C1-4 alkyl, heterocyclyl-C1-4 alkoxy, aryl-C2-10 alkenyl, heteroaryl-C2-10 alkenyl, (un)substituted NH2, carbamoyl, or SO3H, etc.; m, n = 1-3], which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared The chemokine-mediated disease is selected from psoriasis or atopic dermatitis, ***asthma***, chronic obstructive pulmonary disease, adult respiratory distress syndrome, arthritis, inflammatory bowel disease, Crohn's disease, ulcerative colitis, septic shock, endotoxic shock, gram neg. sepsis, toxic shock syndrome, stroke, cardiac and renal reperfusion injury, glomerulo-nephritis, thrombosis, Alzheimer's disease, graft vs. host reaction, and allograft rejections. Thus, 1.19 mmol Me 4-amino-3-hydroxybenzoate was added to a solution of 1.19 mmol Ph isocyanate in toluene and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4-(methoxycarbonyl)phenyl]-N'-phenylurea.

IC ICM A61K031-17

CC 25-21 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

ST phenylurea prepn interleukin 8 receptor antagonist; psoriasis treatment diphenylurea; atopic dermatitis treatment diphenylurea; ***asthma*** treatment diphenylurea; chronic obstructive pulmonary disease treatment diphenylurea; adult respiratory distress syndrome treatment diphenylurea; arthritis treatment diphenylurea; inflammatory bowel disease treatment diphenylurea; Crohn disease treatment diphenylurea; ulcerative colitis treatment diphenylurea; septic shock treatment diphenylurea; endotoxic shock treatment diphenylurea; gram neg sepsis treatment diphenylurea; toxic shock syndrome treatment diphenylurea; cardiac renal reperfusion injury treatment diphenylurea; glomerulo nephritis treatment diphenylurea; thrombosis treatment diphenylurea; Alzheimer disease treatment diphenylurea; graft vs host reaction treatment diphenylurea; allograft rejection treatment diphenylurea; stroke treatment diphenylurea

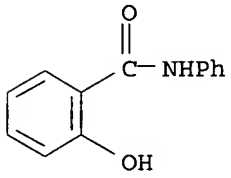
IT 86-84-0, 1-Naphthyl isocyanate ***87-17-2***, 2-Phenylaminocarbonylphenol 88-67-5, 2-Iodobenzoic acid 90-43-7, 2-Phenylphenol 91-93-0 95-54-5, o-Phenylenediamine, reactions 95-55-6, 2-Aminophenol 98-09-9, Phenylsulfonyl chloride 98-17-9, α,α,α-Trifluoro-m-cresol 99-56-9, 4-Nitro-1,2-phenylenediamine 99-57-0, 5-Nitro-2-hydroxyaniline 100-46-9, Benzylamine, reactions 103-71-9, Phenyl isocyanate, reactions 106-40-1, 4-Bromoaniline 116-63-2 117-77-1, 2-Hydroxy-3-aminoanthraquinone 117-99-7 121-51-7, 3-Nitrobenzenesulfonyl chloride 121-60-8, 4-Acetamidophenylsulfonyl chloride 121-88-0, 2-Amino-5-nitrophenol 124-38-9, Carbon dioxide, reactions 137-07-5, 2-Aminothiophenol 274-09-9, 1,3-Benzodioxole 320-76-3 329-01-1, 3-Trifluoromethylphenyl isocyanate 385-01-3, 2-Nitro-3-fluorophenol 394-31-0, 2-Amino-5-hydroxybenzoic acid 394-33-2, 4-Fluoro-2-nitrophenol 400-98-6, 4-Amino-3-nitrobenzotrifluoride 444-30-4, 2-Trifluoromethylphenol 446-36-6, 5-Fluoro-2-nitrophenol 463-71-8, Thiophosgene 534-85-0, 2-Hydroxy-3-aminobenzoic acid 544-92-3, Copper(I) cyanide 570-23-0, 2-Anilinoaliline 576-24-9, 2,3-Dichlorophenol 580-51-8, 3-Phenylphenol 603-87-2, 2-Hydroxy-3-nitroaniline 609-89-2, 4,6-Dichloro-2-nitrophenol 611-20-1, 2-Cyanophenol 614-68-6, 2-Methylphenyl isocyanate 615-36-1, 2-Bromoaniline 618-45-1, 3-Isopropylphenol 620-17-7, 3-Ethylphenol

644-35-9, 2-Propylphenol 700-87-8, 2-Methoxyphenyl isocyanate 776-04-5, 2-(Trifluoromethyl)benzenesulfonyl chloride 837-95-6, 2-Nitro-4-(trifluoromethyl)benzenesulfonyl chloride 873-62-1, 3-Cyanophenol 1548-13-6, 4-Trifluoromethylphenyl isocyanate 1592-00-3, 2-Bromophenyl isocyanate 1623-92-3, 4-Phenoxyphenylsulfonyl chloride 1762-95-4, Ammonium thiocyanate 1899-93-0, 3-Methylbenzenesulfonyl chloride 1939-99-7, Benzylsulfonyl chloride 2237-30-1, 3-Cyanoaniline 2243-42-7, 2-Phenoxybenzoic acid 2285-12-3, 2-Trifluoromethylphenyl isocyanate 2374-03-0, 3-Hydroxy-4-aminobenzoic acid 2493-02-9, 4-Bromophenyl isocyanate 2612-57-9, 2,4-Dichlorophenyl isocyanate 2834-92-6, 1-Amino-2-hydroxynaphthalene 2835-98-5, 2-Hydroxy-4-methylaniline 3272-08-0, 2-Nitro-4-cyanophenol 3320-83-0, 2-Chlorophenyl isocyanate 3320-86-3, 2-Nitrophenyl isocyanate 3470-49-3, 5-Hydroxy-1-indanone 4091-26-3, Styrylsulfonyl chloride 5395-71-1, 2-Ethoxyphenyl isocyanate 5417-63-0, 3-Amino-2-hydroxynaphthalene 6344-59-8, 1-Hydroxy-2-nitrofluorene 7664-41-7, Ammonia, reactions 13020-57-0, 3-Hydroxybenzophenone 13360-57-1, Dimethylsulfamoyl chloride 14755-02-3 16629-19-9, 2-Thiophenesulfonyl chloride 16744-98-2, 2-Fluorophenyl isocyanate 17337-13-2, 2-Phenylphenyl isocyanate 17573-92-1, 3-Methoxythiophene 17802-02-7, 3-Chloro-2-nitrophenol 18162-48-6, tert-Butyldimethylsilyl chloride 18493-15-7 18704-37-5, 8-Quinolinesulfonyl chloride 18908-07-1, 3-Methoxyphenyl isocyanate 20513-43-3 21286-54-4, (+)-10-Camphorsulfonyl chloride 23095-31-0, 3,4-Dimethoxyphenylsulfonyl chloride 24615-22-3 26386-88-9, Diphenylphosphoryl azide 26628-22-8, Sodium azide 32315-10-9, Triphosgene 35821-29-5 39234-86-1 39262-22-1, (-)-10-Camphorsulfonyl chloride 40398-01-4, 2-Chloro-6-methylphenyl isocyanate 40411-25-4, 2-Ethylphenyl isocyanate 41195-90-8, 2,3-Dichlorophenyl isocyanate 43115-40-8, 2-Amino-4-(ethylsulfonyl)phenol 52260-30-7, 2-Methylthiophenyl isocyanate 55076-90-9, 2,4-Dibromophenyl isocyanate 63435-16-5, Methyl 4-amino-3-hydroxybenzoate 65295-69-4, 2,6-Difluorophenyl isocyanate 69812-29-9, 2-Acetamido-4-methyl-5-thiazolesulfonyl chloride 82419-26-9, 2,3-Difluoro-6-nitrophenol 93254-81-0, 2-Benzyloxybenzophenone 99968-81-7, 3-Iodo-2-hydroxyaniline 126714-85-0, 2,3-Dichlorothiophene-5-sulfonyl chloride 146224-62-6, 5-Aminocarbonyl-2-aminophenol 182500-26-1, 2-Trifluoromethoxyphenyl isocyanate 182500-27-2, 2-Amino-5,6-diphenylphenol 182500-28-3, 2-Nitro-5-methyl-4-bromophenol 182500-29-4 182500-30-7, 3,5,6-Trifluoro-2-hydroxyaniline 182500-31-8, 4-Trifluoromethyl-3-fluoro-2-hydroxyaniline 183513-64-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

IT *87-17-2*, 2-Phenylaminocarbonylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

RN 87-17-2 HCAPLUS

CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



L101 ANSWER 32 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:331571 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 125:75309
TITLE: Identification of novel thiocarboxanilide derivatives that suppress a variety of drug-resistant mutant human immunodeficiency virus type 1 strains at a potency similar to that for wild-type virus
AUTHOR(S): Balzarini, J.; Brouwer, W. G.; Dao, D. C.; Osika, E. M.; De Clercq, E.
CORPORATE SOURCE: Rega Inst. Med. Res., Katholieke Univ., Louvain, B-3000, Belg.
SOURCE: Antimicrobial Agents and Chemotherapy (*1996*), 40(6), 1454-1466
CODEN: AMACCQ; ISSN: 0066-4804
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A large variety of carboxanilide and thiocarboxanilide derivs. in which the original oxathiin or aliphatic moieties present in the prototype compds. UC84 and UC38 were replaced by an (un)substituted furanyl, thienyl, Ph, or pyrrole entity have been evaluated for activity against wild-type human immunodeficiency virus type 1 strain IIIB [*HIV*-1(IIIB)] and a series of mutant virus strains derived thereof. The mutant viruses contained either the Leu-100→Ile, Lys-103→Asn, Val-106→Ala, Glu-138→Lys, Tyr-181→Cys, or Tyr-188→Leu mutation in their reverse transcriptase. Several 3-(2-methylfuranyl)- and 3-(2-methylthienyl)-thiocarboxanilide ester, (thio)ether, and oxime ether derivs. showed exquisitely potent antiviral activity against wild-type *HIV*-1 (50% effective concentration, 0.009 to 0.021 μM). The pentenyl-ethers of the 2-methylfuranyl and 2-methylthienyl derivs. (i.e., 313, N-[4-chloro-3-(3-methyl-2-butenyloxy)phenyl]-2-methyl-3-furancarbothiomade or UC-781, and 314, N-[4-chloro-3-(3-methyl-2-butenyloxy)phenyl]-2-methyl-3-thiophenecarbothioamide or UC-82) proved virtually equally inhibitory for wild-type and the Ile-100, Ala-106, and Lys-138 mutant virus strains (50% effective concentration, 0.015 to 0.021 μM). Their inhibitory effect against the Asn-103 and Cys-181 reverse transcriptase mutant virus strains was decreased only four- to sevenfold compared with wild-type virus. UC-781 and UC-82 should be considered potential candidate drugs for the treatment of *HIV*-1-infected individuals.

CC 1-3 (Pharmacology)
ST structure thiocarboxanilide deriv antiviral resistant *HIV1*
IT Drug resistance
Virucides and Virustats
(thiocarboxanilide derivs. structure-related suppression of drug-resistant mutant *HIV*-1 strain)
IT ***Virus, animal***
(***human immunodeficiency 1***, thiocarboxanilide derivs. structure-related suppression of drug-resistant mutant *HIV*-1 strain)
IT Molecular structure-biological activity relationship
(virucidal, thiocarboxanilide derivs. structure-related suppression of drug-resistant mutant *HIV*-1 strain)
IT 135812-51-0 135812-52-1 135812-55-4 135812-56-5 135812-68-9
135813-03-5 135813-04-6 135813-05-7 135813-09-1 135813-46-6
165391-80-0 165391-81-1 165391-82-2 165391-83-3 165391-84-4
172998-56-0 172998-57-1 172998-58-2 172998-59-3 172998-60-6

172998-62-8 172998-75-3 172998-76-4 172998-77-5 173046-03-2
173046-05-4 178869-90-4 178869-91-5 178869-92-6 178869-93-7
178869-94-8 178869-95-9 178869-96-0 178869-97-1 178869-98-2
178869-99-3 178870-00-3 178870-01-4 178870-02-5 178870-03-6
178870-04-7 178870-05-8 178870-06-9 178870-07-0 178870-08-1
178870-09-2 178870-10-5 178870-11-6 178870-12-7
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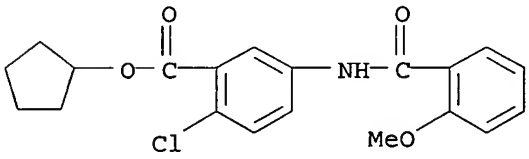
178870-18-3 178870-19-4 178870-20-7 178870-21-8 178870-22-9
178870-23-0 178870-24-1 178870-25-2 178870-26-3 178870-27-4
178870-28-5 178870-29-6 178870-30-9 178870-31-0 178870-32-1
178870-33-2 178870-34-3 178870-35-4 178870-36-5 178870-37-6
178870-38-7 178870-39-8 178870-40-1 178870-41-2 178870-42-3
178870-43-4 178870-44-5 178870-45-6 178870-46-7 178870-47-8
178870-48-9 178870-49-0 178870-50-3 178870-51-4 178870-52-5
178870-53-6 178870-54-7 178870-55-8 180034-55-3 180034-56-4
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); PRP (Properties); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(thiocarboxanilide derivs. structure-related suppression of drug-resistant mutant ***HIV***-1 strain)

IT ***178870-09-2***
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); PRP (Properties); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(thiocarboxanilide derivs. structure-related suppression of drug-resistant mutant ***HIV***-1 strain)

RN 178870-09-2 HCAPLUS

CN Benzoic acid, 2-chloro-5-[(2-methoxybenzoyl)amino]-, cyclopentyl ester (9CI) (CA INDEX NAME)



L101 ANSWER 33 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:967831 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 124:219374
TITLE: Structure-activity and cross-resistance evaluations of a series of human immunodeficiency virus type 1-specific compounds related to oxathiin carboxanilide
AUTHOR(S): Buckheit, Robert W., Jr.; Kinjerski, Tracy L.; Fliakas-Boltz, Valerie; Russell, Julie D.; Stup, Tracy L.; Pallansch, Luke A.; Brouwer, Walter G.; Dao, Dong C.; Harrison, W. Ashley; et al.
CORPORATE SOURCE: Virol. Res. Group, Southern Res. Inst.-Frederick Res. Cent., Frederick, MD, 21701, USA
SOURCE: Antimicrobial Agents and Chemotherapy (***1995***), 39(12), 2718-27
CODEN: AMACCQ; ISSN: 0066-4804
PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of compds. related to the nonnucleoside reverse transcriptase (RT) inhibitor (NNRTI) oxathiin carboxanilide (UC84) were evaluated for activity against the human immunodeficiency virus (***HIV***) to determine structural requirements for anti-***HIV*** activity. Twenty-seven compds. representative of the more than 400 Uniroyal Chemical Company (UC) compds. were evaluated for structure-activity relationships. Several of the compds. evaluated were highly active, with 50% effective concns. in the nanomolar range and therapeutic indexes of >1,000. Highly synergistic anti-***HIV*** activity was observed for each compound when used in combination with 3'-azido-3'-deoxythymidine; additive to slightly synergistic interactions were observed with the compds. used in combination with dideoxycytidine. In combination with the NNRTI costatolide, only UC38 synergistically inhibited ***HIV*** type 1. Residues in the RT which, when mutated, impart resistance to the carboxyanilide compds. were defined by evaluation of the UC compds. against a panel of NNRTI-resistant virus isolates selected in cell culture, against virus variants with site-directed mutations, and against RTs containing defined single amino acid changes. The mutations included changes in RT amino acids 100, 101, 103, 106, 108, and 181. The results with isolates selected in cell culture indicate that the carboxanilide compds. interact with the RT at two vulnerable sites, selecting UC-resistant virus isolates with the Y-to-C mutation at position 181 (Y181C) or the L100I substitution. A resistant virus isolate containing both Y181C and K101E amino acid changes and another with both Y181C and V106A mutations were isolated. In combination with calanolide A, an NNRTI which retains activity against virus isolates with the single Y181C mutation, UC10 rapidly selected a virus isolate with the K103N mutation. The merits of selecting potential candidate anti-***HIV*** agents to be used in rational combination drug design as part of an armamentarium of highly active anti-***HIV*** compds. are discussed.

CC 1-3 (Pharmacology)

ST structure resistance oxathiin carboxanilide analog virucide; ***HIV*** virucide interaction oxathiin carboxanilide analog

IT Virucides and Virustats
(structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT Drug interactions
(additive, structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT Drug resistance
(cross-, structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT Drug interactions
(synergistic, structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT Molecular structure-biological activity relationship
(virucidal, structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

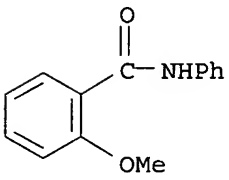
IT ***6833-21-2*** 7022-48-2, NSC 628536 135812-04-3, Oxathiin carboxanilide 135812-34-9, UC38 135812-51-0, UC 25 163464-32-2, NSC 632780 163464-34-4, NSC 638521 165391-81-1, UC 68 165549-68-8, NSC 645542 165549-69-9, UC 581 165549-92-8, UC 33 172998-55-9, NSC 630922 172998-56-0, UC 05 172998-57-1, UC 10 172998-58-2, UC 57 172998-59-3, UC 30 172998-60-6, UC 71 172998-61-7, UC 939 172998-62-8, UC 79 172998-75-3, UC 538 172998-76-4, UC 80 172998-77-5, UC 20 173046-03-2, UC 69 173046-05-4, UC 70

174764-83-1, UC 77
RL: PRP (Properties); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT 7481-89-2, Dideoxycytidine 30516-87-1, 3'-Azido-3'-deoxythymidine 63023-58-5, Costatolide 142632-32-4, Calanolide A
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

IT ***6833-21-2***
RL: PRP (Properties); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(structure-activity and cross-resistance evaluations of series of ***HIV***-1-specific compds. related to oxathiin carboxanilide)

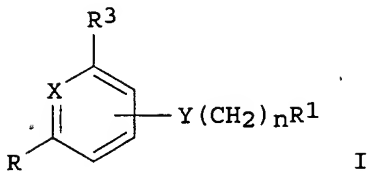
RN 6833-21-2 HCAPLUS
CN Benzamide, 2-methoxy-N-phenyl- (9CI) (CA INDEX NAME)



L101 ANSWER 34 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:905394 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 123:313563
TITLE: Preparation of N-(phenylmethyl)hexanamides and analogs as protein kinase C inhibitors
INVENTOR(S): Daines, Robert A.
PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9517888	A1	19950706	WO 1994-US14684		19941220 <--
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KP, KR, KZ, LK, MG, MN, MW, NO, NZ, PT, RO, RU, SD, SI, SK, UA, US, VN					
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
AU 9514411	A1	19950717	AU 1995-14411		19941220 <--
EP 738144	A1	19961023	EP 1995-906035		19941220 <--
R: BE, CH, DE, FR, GB, IT, LI, NL					
JP 09507846	T2	19970812	JP 1994-518118		19941220 <--
ZA 9410318	A	19950801	ZA 1994-10318		19941227 <--
PRIORITY APPLN. INFO.:			US 1993-176357	A	19931230 <--
			WO 1994-US14684	W	19941220 <--

OTHER SOURCE(S): MARPAT 123:313563
GI



I

AB Title compds. [I; R = R4R5N(CH2)mZEpZ1; E = CHR9; R1 = H, alkyl, (hetero)aryl, etc.; R3 = H, C.tplbond.CR6; (CH2)kR6; R4,R5 = H or alkyl; NR4R5 = heterocyclyl; R6 = aryl, alkoxycarbonyl, (alkanoyl)amino, etc.; R9 = H, alkyl, alkoxy, etc.; X = CH or N; Y = CH2, O, S, etc.; Z = CH2, (hetero)arylene, etc.; Z1 = CONR2, NR2CO; R2 = H or alkyl; k,m = 0-10; n = 6-20; p = 0 or 1] were prepared Thus, 2-(HO)C6H4CHO was converted in 2 steps to 2-[Me(CH2)11O]C6H4CH2NHMe which was amidated by Nα,Nε-di-tert-butoxycarbonyl-L-lysine N-hydroxysuccinimide ester to give, after deprotection, (S)-2-[Me(CH2)11O]C6H4CH2NMeCOCH(NH2)(CH2)4NH2.2HCl. I had IC50 of 0.001-150μM for inhibition of protein kinase C.

IC ICM A61K031-165
ICS A61K031-24; A61K031-44; A61K031-495; A61K031-535; C07C229-38; C07C235-50; C07C237-08; C07D213-64; C07D241-04; C07D265-30

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1

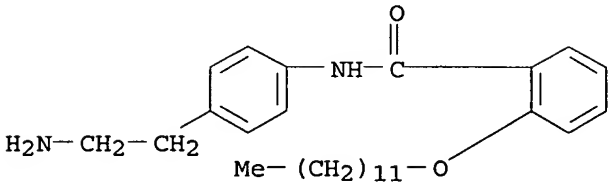
IT Inflammation inhibitors
Neoplasm inhibitors
(preparation of N-(phenylmethyl)hexanamides and analogs as protein kinase C inhibitors)

IT 170016-87-2P 170016-88-3P 170016-89-4P 170016-90-7P 170016-91-8P
170016-92-9P 170016-93-0P 170016-94-1P 170016-95-2P 170016-96-3P
170016-97-4P 170016-98-5P 170016-99-6P 170017-00-2P 170017-01-3P
170017-02-4P 170017-03-5P 170017-04-6P 170017-05-7P
170017-06-8P 170017-07-9P 170017-08-0P 170017-09-1P
170017-10-4P 170017-11-5P 170017-12-6P 170017-13-7P 170017-14-8P
170017-15-9P 170017-16-0P 170017-17-1P 170017-18-2P 170017-19-3P
170017-20-6P 170017-21-7P 170017-22-8P 170017-23-9P 170017-24-0P
170017-25-1P ***170017-26-2P*** 170017-27-3P ***170017-28-4P***
170017-29-5P 170017-30-8P 170017-31-9P 170017-32-0P
170017-33-1P 170017-34-2P 170017-35-3P 170017-36-4P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(phenylmethyl)hexanamides and analogs as protein kinase C inhibitors)

IT ***170017-06-8P 170017-26-2P 170017-28-4P***
170017-29-5P
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-(phenylmethyl)hexanamides and analogs as protein kinase C inhibitors)

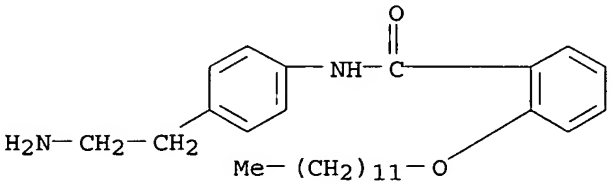
RN 170017-06-8 HCAPLUS
CN Benzamide, N-[4-(2-aminoethyl)phenyl]-2-(dodecyloxy)-, monohydrochloride

(9CI) (CA INDEX NAME)

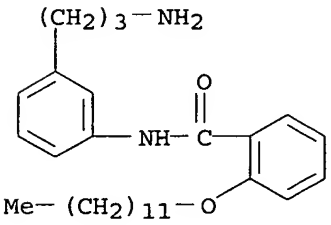


● HCl

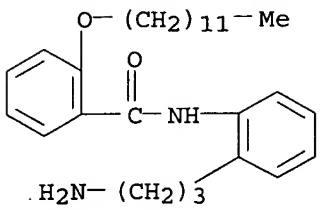
RN 170017-26-2 HCAPLUS
CN Benzamide, N-[4-(2-aminoethyl)phenyl]-2-(dodecyloxy)- (9CI) (CA INDEX NAME)



RN 170017-28-4 HCAPLUS
CN Benzamide, N-[3-(3-aminopropyl)phenyl]-2-(dodecyloxy)- (9CI) (CA INDEX NAME)



RN 170017-29-5 HCAPLUS
CN Benzamide, N-[2-(3-aminopropyl)phenyl]-2-(dodecyloxy)- (9CI) (CA INDEX NAME)



L101 ANSWER 35 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:858623 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 123:256357
TITLE: Preparation of anthranilic acid amide derivative as cyclic guanosine monophosphate-phosphodiesterase inhibitors
INVENTOR(S): Ozaki, Fumihiro; Ishibashi, Keiji; Ikuta, Hironori; Ishihara, Hiroki; Souda, Shigeru
PATENT ASSIGNEE(S): Japan
SOURCE: PCT Int. Appl., 204 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
WO 9518097	A1	19950706	WO 1994-JP2262		19941227	<--
W: AU, CA, CN, FI, HU, KR, NO, NZ, RU, US						
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE						
CA 2155662	AA	19950706	CA 1994-2155662		19941227	<--
AU 9512824	A1	19950717	AU 1995-12824		19941227	<--
AU 694465	B2	19980723				
EP 686625	A1	19951213	EP 1995-903999		19941227	<--
EP 686625	B1	19990526				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE						
CN 1118595	A	19960313	CN 1994-191311		19941227	<--
JP 08188563	A2	19960723	JP 1994-336920		19941227	<--
HU 74450	A2	19961230	HU 1995-2512		19941227	<--
RU 2128644	C1	19990410	RU 1995-120194		19941227	<--
AT 180468	E	19990615	AT 1995-903999		19941227	<--
FI 9503968	A	19951019	FI 1995-3968		19950823	<--
NO 9503305	A	19951025	NO 1995-3305		19950823	<--
US 5716993	A	19980210	US 1995-507476		19950914	<--
PRIORITY APPLN. INFO.:			JP 1993-347092	A	19931227	<--
			JP 1994-299110	A	19941109	<--
			WO 1994-JP2262	W	19941227	<--

OTHER SOURCE(S): MARPAT 123:256357
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Anthranilamide derivs. [I; R1, R2, R3, R4 = H, halo, OH, (halo)alkyl, (halo)alkoxy, nitro, hydroxyalkyl, cyano, (CH2)pNR9R10, S(O)qR13,

(un)protected CO2H, (un)substituted tetrazolyl, CONH2, pyrazolyl, or imidazolyl; or adjacent two substituents selected from R1 - R4 together with the C atoms bonded to them forms a ring; wherein R9, R10 = H, (halo)alkyl, arylalkyl, heteroarylalkyl, acyl, (un)protected CO2H; or NR9R10 forms a ring; p = 0, 1-6; R13 = H, (halo)alkyl; q = 0, 1-2; R5, R6 = H, halo, OH, cyano, (halo)alkyl, (halo)alkoxy; or R5 and R6 together with the C atoms bonded to them form cycloalkane, oxolane, 1,3-dioxolane, or 1,4-dioxane ring; W = N, CH; R7, R8 = H, (halo)alkyl; or R1 and R7 together with the C atoms bonded to them form a ring optionally containing other N, O, or S atom; A = H, (halo)alkyl, X(CH2)mZ; wherein X = CO, CS, CH2, SO2; Z = OH, (halo)alkoxy, cyano, halo, etc.; Y = O, S; n = 0, 1-6] or pharmacol. acceptable salts thereof are prepared These compds. are useful for the treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and ***asthma***. Thus, 2-nitro-5-chlorobenzoic acid was refluxed with SOCl2 in benzene for 4 h and concentrated to give 2-nitro-5-chlorobenzoyl chloride which was amidated with piperonylamine in the presence of Et3N in THF to give a benzamide (II; R = NO2). This compound was reduced by Fe powder in a mixture of AcOH, H2O, and MeOH under gentle refluxing to give, after concentration and treatment with concentrated HCl in EtOH, N-piperonylanthranilamide derivative II. HCl (R = NH2). An anthranilamide derivative (III) showed IC50 of 0.4 nM against cyclic guanosine monophosphate-phosphodiesterase preparation from pig aorta.

IC ICM C07C237-30
ICS C07C237-42; C07D265-26; C07D317-60; C07D405-12; A61K031-36; A61K031-44; A61K031-445; A61K031-495

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 7, 27, 28

ST anthranilic acid amide prepn treatment hypertension; cyclic guanosine monophosphate phosphodiesterase inhibitor; ischemic heart disease treatment anthranilamide; piperonylanthranilamide treatment angina pectoris; pulmonary hypertension treatment anthranilamide; heart failure treatment anthranilamide; ***asthma*** treatment anthranilamide; cGMP phosphodiesterase treatment anthranilamide

IT Antihypertensives
(preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors for treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and ***asthma***)

IT Heart, disease
(angina pectoris, preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors for treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and ***asthma***)

IT Bronchodilators
(***antiasthmatics***, preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors for treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and ***asthma***)

IT Heart, disease
(failure, preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors for treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension, heart failure, and ***asthma***)

IT Heart, disease
(ischemia, preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors for treatment of ischemic heart disease, angina pectoris, hypertension, pulmonary hypertension,

heart failure, and ***asthma***)

IT 169043-28-1P 169043-29-2P 169043-30-5P 169043-31-6P 169043-32-7P
169043-33-8P 169043-34-9P 169043-35-0P 169043-36-1P 169043-37-2P
169043-38-3P 169043-39-4P 169043-40-7P 169043-41-8P 169043-42-9P
169043-43-0P 169043-44-1P 169043-45-2P 169043-46-3P 169043-47-4P
169043-48-5P 169043-49-6P 169043-50-9P 169043-51-0P 169043-52-1P
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169043-58-7P 169043-59-8P 169043-60-1P 169043-61-2P 169043-62-3P
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169043-93-0P 169043-94-1P 169043-95-2P 169043-96-3P 169043-97-4P
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169044-57-9P 169044-58-0P 169044-59-1P 169044-60-4P 169044-61-5P
169044-62-6P 169044-63-7P 169044-64-8P 169044-65-9P 169044-66-0P
169044-67-1P 169044-68-2P

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors)

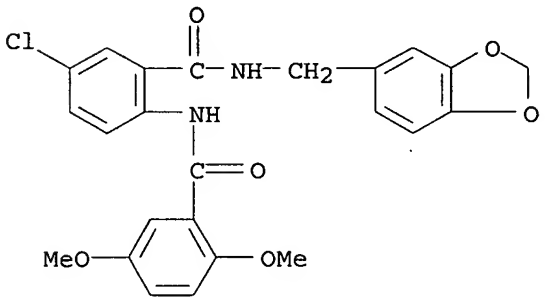
IT ***169044-55-7P***

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); SPN (Synthetic preparation); ***THU (Therapeutic use)***; BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of anthranilamide derivs. as cyclic guanosine monophosphate-phosphodiesterase inhibitors)

RN 169044-55-7 HCAPLUS

CN Benzamide, N-[2-[[(1,3-benzodioxol-5-ylmethyl)amino]carbonyl]-4-chlorophenyl]-2,5-dimethoxy- (9CI) (CA INDEX NAME)



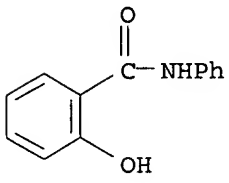
L101 ANSWER 36 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:641364 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 119:241364
TITLE: Method for the prescreening of drugs targeted to the V3 hypervariable loop of the *HIV*-1 envelope glycoprotein gp 120
INVENTOR(S): Neurath, Alexander R.; Strick, Nathan; Haberfield, Paul; Jiang, Shibo
PATENT ASSIGNEE(S): USA
SOURCE: U.S., 30 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5230998	A	19930727	US 1991-735640	19910725 <--
PRIORITY APPLN. INFO.:			US 1991-735640	19910725 <--

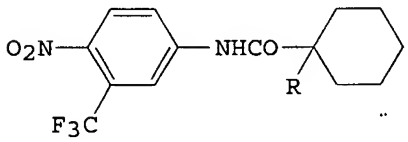
AB A method for the rapid screening of a drug (e.g. porphyrin derivative) targeted to the V3 hypervariable loop of the human immunodeficiency virus type 1 or type 2 envelope glycoprotein gp 120 comprises measuring the inhibitory effect of the drug on the interaction between gp 120 (or an antigen comprising the V3 hypervariable loop of *HIV* 1 gp 120 or *HIV* 2 gp 120) and antibodies specific for the V3 hypervariable loop.

IC ICM G01N033-545
INCL 435007100
CC 1-1 (Pharmacology)
ST *HIV* virus inhibitor screening binding interaction
IT Amines, biological studies
Chlorophyllins
Phenols, biological studies
Quaternary ammonium compounds, biological studies
Sulfonates
Tannins
RL: PRP (Properties)
(screening of, as *HIV* virus inhibitor, inhibition of interaction between *HIV*-1 or *HIV*-2 gp 120 and anti-V3 hypervariable loop antibody in)
IT Antibodies
RL: BIOL (Biological study)
(to V3 hypervariable loop, *HIV*-1 of *HIV*-2 gp 120 interaction with, in *HIV* virus inhibitor screening)
IT Porphyrins
RL: BIOL (Biological study)
(carboxy, dihydrochloride salt, screening of, as *HIV* virus inhibitor, inhibition of interaction between *HIV*-1 or *HIV*-2 gp 120 and anti-V3 hypervariable loop antibody in)
IT Sialoglycoproteins
RL: BIOL (Biological study)
(gp120env, anti-V3 hypervariable loop antibody interaction with, in *HIV* virus inhibition screening)
IT Virus, animal
(human immunodeficiency 1, gp 120, anti-V3 hypervariable loop antibody interaction with, in *HIV* virus inhibitor screening)

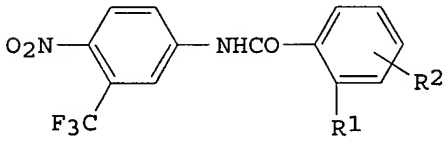
IT ***87-17-2***, Salicylanilide
RL: PRP (Properties)
(screening of, as ***HIV*** virus inhibitor, inhibition of interaction between ***HIV***-1 or ***HIV***-2 gp 120 and anti-V3 hypervariable loop antibody in)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



L101 ANSWER 37 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1988:610640 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 109:210640
TITLE: Development of potential nonsteroidal antiandrogens: N-[4-nitro-3-(trifluoromethyl)phenyl]cyclohexanecarboxamides and -benzamides and N-(3,4-dichlorophenyl)- and N-(3,4,5-trichlorophenyl)benzamides
AUTHOR(S): Humm, Alfred W.; Schneider, Martin R.
CORPORATE SOURCE: Inst. Pharm., Univ. Regensburg, Regensburg, D-8400, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (***1988***), 321(7), 419-22
CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 109:210640
GI



I



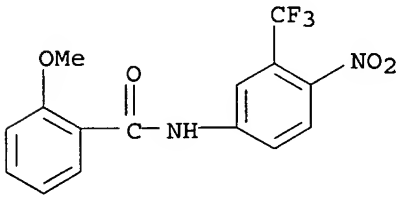
II

AB Title compds. I (R = H, Br, OH), II (R1 = H, R2 = H, 3-OMe, 4-OMe; R1 = OMe, R2 = H, 3-OMe, 4-OMe, 5-OMe, 6-OMe) and 2-MeOC6H4CONHC6H3Cl2R3-3,4,5 (III R3 = H, Cl) were prepared by amidation of the acid chlorides. I (R = OH) had a greater binding affinity for the androgen receptor than

IT Virus, animal
(human immunodeficiency 2, gp 120, anti-V3 hypervariable loop antibody interaction with, in ***HIV*** virus inhibitor screening)

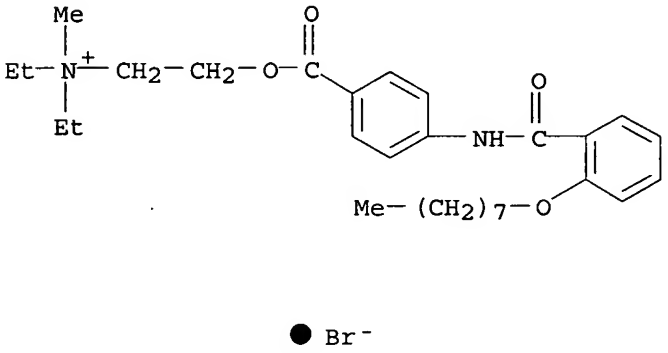
IT 50-76-0, Actinomycin D 58-15-1, Aminopyrine 65-49-6 68-19-9, Vitamin B12 69-72-7, biological studies 76-59-5, Bromothymol blue 76-61-9, Thymol blue 77-09-8, Phenolphthalein 80-09-1, 4,4'-Dihydroxydiphenylsulfone 81-61-8, Quinalizarin 81-88-9, Rhodamine B 82-45-1, 1-Aminoanthraquinone 84-48-0, 2-Anthraquinonesulfonic acid ***87-17-2***, Salicylanilide 89-57-6 90-01-7, Saligenin 90-20-0 90-30-2, N-Phenyl-1-naphthylamine 90-41-5, 2-Aminobiphenyl 90-44-8, Anthrone 92-66-0, 4-Bromobiphenyl 92-67-1, [1,1'-Biphenyl]-4-amine 92-69-3, 4-Phenylphenol 92-87-5, Benzidine 92-88-6, [1,1'-Biphenyl]-4,4'-diol 92-92-2, 4-Biphenylcarboxylic acid 92-93-3 94-67-7, Salicylaldoxime 101-53-1 103-32-2, N-Phenylbenzylamine 115-40-2, Bromocresol purple 115-86-6 116-63-2 117-79-3, 2-Aminoanthraquinone 118-32-1 118-55-8, Phenyl salicylate 122-39-4, Diphenylamine, biological studies 129-03-3 130-95-0, Quinine 131-27-1 136-95-8, 2-Benzothiazolamine 143-66-8, Sodium tetraphenylborate 143-74-8, Phenol red 148-25-4, 4,5-Dihydroxynaphthalene-2,7-disulfonic acid 153-78-6, 2-Aminofluorene 260-94-6, Acridine 294-90-6, Cyclen 298-46-4, Carbamazepine 298-96-4, 2,3,5-Triphenyl-2H-tetrazolium chloride 314-13-6 321-60-8 479-61-8, Chlorophyll a 482-89-3, Indigo 484-47-9, 2,4,5-Triphenylimidazole 493-77-6, 2,4,6-Triphenyl1,3,5-triazine 519-62-0, Chlorophyll b 548-62-9, Crystal violet 548-80-1 553-12-8, Protoporphyrin IX 569-64-2, Malachite green 573-58-0 595-91-5, Triphenylacetic acid 610-49-1, 1-Aminoanthracene 613-37-6, 4-Phenylanisole 768-94-5, 1-Adamantanamine 789-47-9, 2-Aminochrysene 791-28-6, Triphenylphosphine oxide 900-91-4, 3,3,3-Triphenylpropionic acid 947-73-9, 9-Phenanthrenamine 975-17-7, 9-Phenyl-2,3,7-trihydroxy-6-fluorone 1137-41-3 1461-15-0, Calcein 1502-03-0, Cyclododecanamine 1528-74-1 1625-84-9 1667-99-8, Chrome azurol S 1689-64-1, 9-Hydroxyfluorene 1733-12-6, Cresol red 2090-82-6, Phenolphthalein diphosphate 2224-32-0, Triphenylphosphonium cyclopentadienylide 2243-76-7 2321-07-5 2443-58-5, 2-Hydroxyfluorene 2693-46-1, 3-Fluoranthenamine 2799-07-7 2834-79-9 2920-38-9, 4-Biphenylcarbonitrile 3218-36-8, 4-Biphenylcarboxaldehyde 3244-88-0 3564-18-9 3878-45-3, Triphenylphosphine sulfide 4383-07-7 4431-00-9, Aurintricarboxylic acid 5443-16-3 5449-84-3 5452-37-9, Cyclooctanamine 5715-76-4 5824-40-8, Tritylamine 5893-05-0, N-Tritylglycine 6571-43-3, 2,3-Cyclododecenopyridine 6638-60-4 6864-20-6, 2,4,6-Triphenylaniline 8004-87-3, Methyl violet 10303-95-4, 1,3-Adamantanediamine 10527-16-9, 10-Chloro-9-anthraldehyde 13074-39-0, 2-Adamantanamine 13862-13-0, 3,5-Diiodosaligenin 13881-91-9, Aminomethanesulfonic acid 14609-54-2 16009-13-5, Hemin 16423-68-0 16568-56-2 16834-13-2 17372-87-1, Eosin y 18928-00-2 19660-77-6, Chlorine e6 21278-45-5 21373-30-8 28059-64-5, 2-Benzylaniline 36951-72-1 39269-10-8, 1,3-Adamantanedicarboxylic acid 47672-25-3 51757-47-2 57618-17-4 58010-91-6 65817-53-0, 1-Amino-7-nitrofluorene 68929-06-6 68938-73-8 69438-84-2 69477-27-6 76079-45-3 79055-30-4 79236-56-9, N-Methyl protoporphyrin IX 82801-91-0 101637-58-5 102747-84-2 119431-30-0 137821-07-9 139979-70-7 150957-19-0 150957-20-3 150957-21-4 150957-22-5 150957-23-6 150957-24-7 150957-25-8 150957-26-9 150957-29-2 150996-91-1 150996-92-2 150996-93-3 151146-05-3
RL: PRP (Properties)
(screening of, as ***HIV*** virus inhibitor, inhibition of interaction between ***HIV***-1 or ***HIV***-2 gp 120 and anti-V3 hypervariable loop antibody in)

hydroxyflutamide II and III were less active.
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 2
IT ***117367-11-0P*** 117367-12-1P 117367-13-2P 117367-14-3P
117367-15-4P 117367-16-5P 117367-17-6P 117367-18-7P 117367-19-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)
IT ***117367-11-0P***
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demethylation of)
RN 117367-11-0 HCAPLUS
CN Benzamide, 2-methoxy-N-[4-nitro-3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)



L101 ANSWER 38 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:197534 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 104:197534
TITLE: Diethylmethyl{2-[p-(o-octyloxybenzamido)benzoyloxy]ethyl}ammonium bromide (I) and diethylmethyl{2-[p-(o-propyloxybenzamido)benzoyloxy]ethyl}ammonium bromide (II)
AUTHOR(S): Dapporto, Paolo; Sega, Alessandro
CORPORATE SOURCE: Dip. Energ., Univ. Firenze, Florence, 50139, Italy
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (***1986***), C42(4), 474-8
CODEN: ACSCEE; ISSN: 0108-2701
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Title compound I is monoclinic, space group P21/c, with a 19.023(6), b 16.767(5), c 9.497(4) Å, and β 94.57(5)°; Z = 4; for dc = 1.239. The final R = 0.079 for 1379 reflections. Title compound II is triclinic, space group P.***hivin***.1, with a 15.929(9), b 8.261(5), c 9.417(6) Å, α 89.916(4), β 96.954(4), and γ 89.188(4)°; Z = 2 for dc = 1.332. The final R = 0.047 for 2114 reflections. The structures of I and II are quite similar: the benzoanilide moieties are nearly planar; the quaternary N side chains show the same trans-trans-gauche trend for the corresponding torsional angles. The only remarkable difference lies in the orientation of their alkyloxy chains. In I the ends of the 2 side chains are spatially closely related giving to the mol. a 'loop' conformation. Atomic coordinates are given.
CC 75-8 (Crystallography and Liquid Crystals)
Section cross-reference(s): 25
IT ***26095-59-0*** 51444-54-3
RL: PRP (Properties)
(structure of)

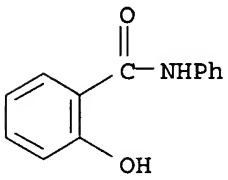
IT *26095-59-0*
RL: PRP (Properties)
(structure of)
RN 26095-59-0 HCAPLUS
CN Ethanaminium, N,N-diethyl-N-methyl-2-[[4-[[2-(octyloxy)benzoyl]amino]benzoyl]oxy]-, bromide (9CI) (CA INDEX NAME)



● Br^-

L101 ANSWER 39 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1986:178084 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 104:178084
TITLE: Structure of N-aromatic amides. II. XC6H4NHCOY
AUTHOR(S): Kashino, Setsuo; Matsushita, Toshiko; Iwamoto, Tetsuyuki; Yamaguchi, Katsuji; Haisa, Masao
CORPORATE SOURCE: Fac. Sci., Okayama Univ., Tsushima, 700, Japan
SOURCE: Acta Crystallographica, Section C: Crystal Structure Communications (*1986*), C42(4), 457-62
CODEN: ACSCEE; ISSN: 0108-2701
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Salicylanilide (X = H, Y = o-HOC6H4) (I) is orthorhombic, space group Pbca, with a 11.018(2), b 24.781(5), and c 7.760(1) Å; dm = 1.33 and dc = 1.337 for Z = 8; final R = 0.050. o-Nitroacetanilide (X = o-NO2, Y = CH3), (II) is monoclinic, space group P21/n, with a 15.507(3), b 4.9576(5), c 10.924(2) Å, and β 97.68(1)°; dm = 1.45 and dc = 1.438 for Z = 4; final R = 0.052. p-Acetamidobenzoic acid (X = p-COOH, Y = CH3), (III) is triclinic, space group P*hivin*.1, with a 6.9858(5), b 12.623(1), c 5.0045(4) Å, α 102.575(6), β 101.837(6), and γ 83.818(6)°; dm = 1.41 and dc = 1.415 for Z = 2; final R = 0.042. The effect of the substituents X and Y on the crystal structure of acetanilides is discussed. The nitro and carboxyl groups dominate the structures, while the role of the amide group is only complementary. In I, the mols. form H-bonded ribbons held together with van der Waals forced to form sheets, which are stacked along b. In II, the mols. stack to form columns with dipole-dipole interactions between the nitro groups.f. The C:O group is not involved in any H bonding. In III, the acid dimers are H bonded to form ribbons. The ribbons form sheets, which are stacked along b. The atomic coordinates are given.
CC 75-8 (Crystallography and Liquid Crystals)
Section cross-reference(s): 25
IT *87-17-2* 552-32-9 556-08-1
RL: PRP (Properties)

(crystal structure of)
IT *87-17-2*
RL: PRP (Properties)
(crystal structure of)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



L101 ANSWER 40 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1979:66509 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 90:66509
TITLE: Potential antitumor agents. 29. Quantitative structure-activity relationships for the antileukemic bisquaternary ammonium heterocycles
AUTHOR(S): Denny, William A.; Atwell, Graham J.; Baguley, Bruce C.; Cain, Bruce F.
CORPORATE SOURCE: Exp. Chemother. Res. Lab., Pew Zealand Cancer Soc., Auckland, N. Z.
SOURCE: Journal of Medicinal Chemistry (*1979*), 22(2), 134-50
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Quant. relations between physicochem. drug properties and antileukemic (L1210) efficacy were examined for a series of bisquaternary ammonium heterocycles employing multiple variable regression anal. The synthesis of these compds. is described. The drug dose necessary to provide a 40% increase in life span and the chemotherapeutic index were independent of toxicity. There was a parabolic relation between agent lipophilic-hydrophilic balance and the percentage increase in mean life span of leukemic animals at the LD10 dose. Relative levels of drug-DNA interaction were obtained by spectrofluorimetric quantitation of drug displacement of DNA-bound ethidium. Extensive quant. structure-activity relations are discussed.
CC 1-3 (Pharmacodynamics)
Section cross-reference(s): 27
ST ***neoplasm*** inhibitor bisquaternary ammonium heterocycle; antileukemic bisquaternary ammonium heterocycle
IT ***Neoplasm*** inhibitors
(bisquaternary ammonium heterocycles)
IT Molecular structure-biological activity relationship
(***neoplasm***-inhibiting, of bisquaternary ammonium heterocycles)
IT 14101-73-6 14120-88-8 14120-89-9 14120-90-2 14120-92-4
14120-94-6 14170-93-5 14242-15-0 14242-18-3 14242-19-4
14357-93-8 14796-58-8 16758-28-4 16758-31-9 16758-32-0
16758-33-1 16760-09-1 16760-11-5 16760-12-6 16760-13-7
16760-14-8 16760-16-0 16760-18-2 16760-21-7 16760-22-8
16760-23-9 16802-49-6 16802-50-9 17794-13-7 18355-45-8
18355-50-5 18355-51-6 18355-52-7 18355-53-8 18355-54-9

18355-56-1 18430-43-8 18430-44-9 18519-35-2 18519-37-4
18519-40-9 18519-41-0 18519-47-6 18519-49-8 18519-50-1
18519-58-9 18519-60-3 18519-63-6 18519-65-8 18519-66-9
18519-67-0 18519-69-2 18520-35-9 18520-36-0 18520-38-2
18520-42-8 18520-43-9 18520-44-0 18520-45-1 18520-46-2
18520-50-8 18520-54-2 18520-56-4 18520-57-5 18520-59-7
19055-86-8 19055-99-3 19056-01-0 19056-03-2 19056-04-3
19056-06-5 19056-07-6 19056-08-7 19056-14-5 19056-21-4
19060-32-3 19060-33-4 19060-34-5 19060-39-0 19060-40-3
19060-42-5 19060-43-6 19060-44-7 ***19060-74-3***
19060-75-4 ***19060-76-5*** 19083-77-3 19083-80-8
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68772-12-3 68772-13-4 68772-15-6 68772-18-9 68772-19-0
68772-21-4 68772-24-7 68772-26-9 68772-27-0 68772-28-1
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68772-40-7 68772-43-0 68772-47-4 68797-91-1 68798-18-5
68967-17-9 68967-21-5 68967-23-7 68992-58-5

RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); BIOL (Biological study)
(antileukemic activity of)

IT ***19060-74-3 19060-75-4 19060-76-5***

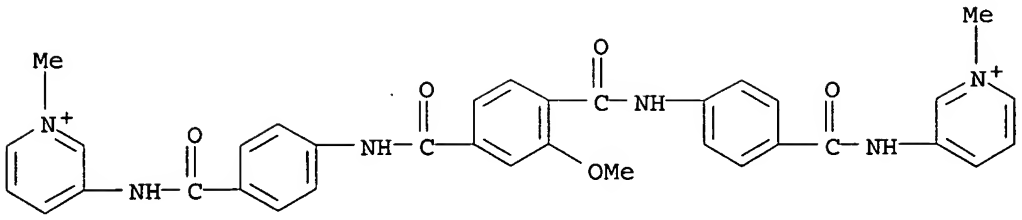
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); BIOL (Biological study)
(antileukemic activity of)

RN 19060-74-3 HCAPLUS

CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-methyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

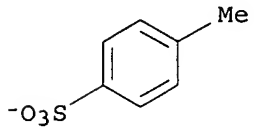
CM 1

CRN 47863-82-1
CMF C35 H32 N6 O5



CM 2

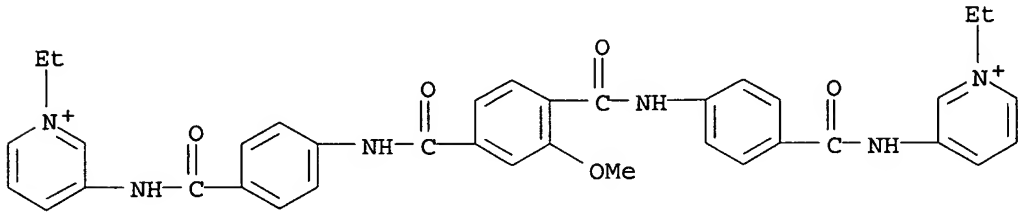
CRN 16722-51-3
CMF C7 H7 O3 S



RN 19060-75-4 HCAPLUS
CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-ethyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

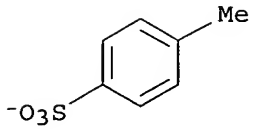
CM 1

CRN 47870-25-7
CMF C37 H36 N6 O5



CM 2

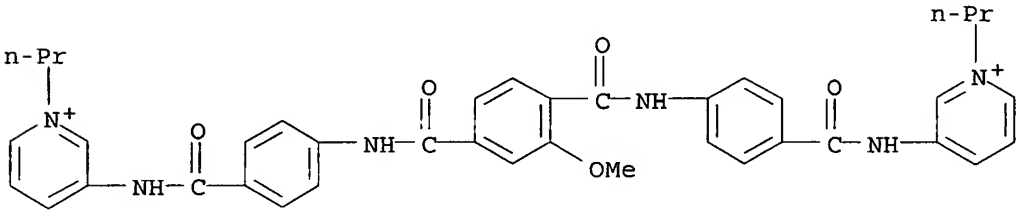
CRN 16722-51-3
CMF C7 H7 O3 S



RN 19060-76-5 HCAPLUS
CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-propyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

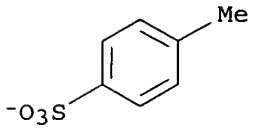
CM 1

CRN 47878-28-4
CMF C39 H40 N6 O5



CM 2

CRN 16722-51-3
CMF C7 H7 O3 S



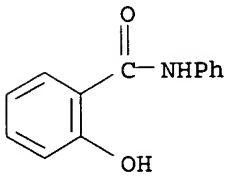
L101 ANSWER 41 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1978:122930 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 88:122930
TITLE: Additives for clothes dryers
INVENTOR(S): Rudy, Jerome; Rapisarda, Anthony A.
PATENT ASSIGNEE(S): Lever Brothers Co., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4012326	A	19770315	US 1971-158090	19710629 <--
US 3972131	A	19760803	US 1972-265124	19720622 <--
US 4238531	A	19801209	US 1977-853663	19771121 <--
US 4327133	A	19820427	US 1980-161639	19800620 <--
PRIORITY APPLN. INFO.:			US 1969-821476	A1 19690502 <--
			US 1971-158090	A1 19710629 <--
			US 1973-376586	A1 19730705 <--
			US 1975-589993	A1 19750624 <--
			US 1977-853663	A3 19771121 <--

OTHER SOURCE(S): MARPAT 88:122930

AB Drying wearing apparel with bodies containing a mixture of ≤95% of an additive, e.g., dimethyldistearylammonium chloride (I) [107-64-2] softening agent in a diluent spreadable under drying conditions in a dryer or drying the apparel in a dryer spray coated with the mixture imparted a finished property to the apparel. Thus, swatches of a fabric and chips containing 10% I and urea were dried together for 45 min to give a uniformly soft fabric.

IC D06M013-46
INCL 252008800
CC 46-4 (Surface Active Agents and Detergents)
IT Paraffin waxes and Hydrocarbon waxes, uses and miscellaneous
RL: USES (Uses)
(ironing ***aids***, for wearing apparel)
IT ***87-17-2D***, bromo derivs.
RL: USES (Uses)
(bactericidal finishing agents, for wearing apparel)
IT ***87-17-2D***, bromo derivs.
RL: USES (Uses)
(bactericidal finishing agents, for wearing apparel)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



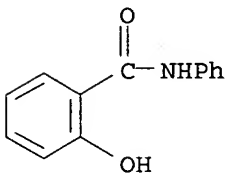
L101 ANSWER 42 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1970:4285 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 72:4285
TITLE: Dispersing agents for dyes and dyeing assistants
INVENTOR(S): Black, William; Paget, Hugh P. D.; Topham, Arthur
PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.
SOURCE: Ger. Offen., 24 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 1902110	A	19690904	DE 1969-1902110	19690116 <--
GB 1239016	A	19710714	GB 1968-2405	19680116 <--
FR 2000311	A5	19690905	FR 1969-702	19690116 <--
CH 509277	A	19710630	CH 1969-509277	19690116 <--
PRIORITY APPLN. INFO.:			GB 1968-2405 A	19680116 <--

AB Dispersing agents for vat or disperse dyes and H2O-insol. dyeing assistants, such as salicylanilide, are prepared by reacting at 160° 1 mole naphthalene (I) with 0.5-1.5 moles PhCH2Cl and 1.0-1.5 moles H2SO4 and then treating the reaction product at 100-105° with HCHO. Thus, a mixture of 256 parts I znc 189 parts PhCH2Cl was stirred at 60°, treated for 30 min. with 221 parts H2SO4, heated to 160°, kept at 160° for 2 hrs., cooled to 100°, treated with 220 parts H2O and 179 parts of an aqueous 35.7% HCHO solution, stirred at 100-5° for 16 hrs., diluted with 200 parts H2O, neutralized with a 30% NaOH solution, and filtered to give a solution (II) with a 43.4% solids content. A mixture of 31 parts C.I. Disperse Yellow 42, 28.6 parts II, and 40.1 parts H2O was ground in a sand-grinder until the particles had an average diameter <4 μ, yielding a paste suitable for dyeing synthetic fibers. This paste (3 parts) diluted with 50 parts H2O, heated at the b.p. for 30 min., and filtered on Whatman Number 4 paper gave practically no residue on the filter.

IC C07C; D06Q
CC 39 (Textiles)
ST dispersing agents dyes; dyes dispersing agents; ***aids*** dispersing agents dyeing; fibers dispersing agents dyeing
IT ***87-17-2***
RL: USES (Uses)
(printing pastes containing, dispersing agents for, from naphthalene sulfonic acid-formaldehyde condensation products)
IT ***87-17-2***
RL: USES (Uses)
(printing pastes containing, dispersing agents for, from naphthalene sulfonic acid-formaldehyde condensation products)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)



L101 ANSWER 43 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1968:85828 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 68:85828
TITLE: Potential antitumor agents. VII. Bisquaternary salts
AUTHOR(S): Atwell, G. J.; Cain, Bruce F.; Seelye, Ralph N.
CORPORATE SOURCE: Cornwall Geriatric Hosp., Auckland, N. Z.
SOURCE: Journal of Medicinal Chemistry (***1968***), 11(2), 300-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The effects of a series of substituents on the biol. activity of a bisquaternary ammonium heterocycle (I) were determined against the L1210 leukemia system in mice.

CC 15 (Pharmacodynamics)

ST AMMONIUM HETEROCYCLES ***TUMORS***; INHIBITORS LEUKEMIA; LEUKEMIA INHIBITORS; ***TUMORS*** AMMONIUM HETEROCYCLES

IT ***Neoplasm*** inhibitors
(bisquaternary ammonium heterocycles as)

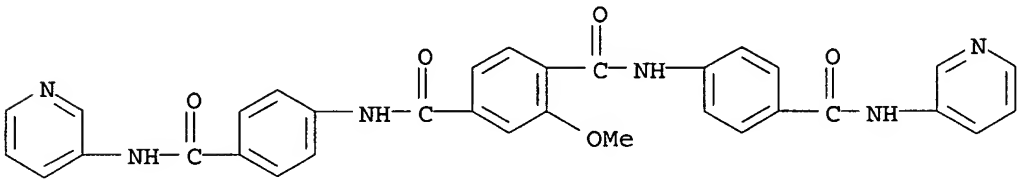
IT Molecular structure-biological activity relationships
(***neoplasm*** inhibiting, of bisammonium heterocycles)

IT 16760-11-5 16760-12-6 16760-13-7 16760-14-8 16760-15-9
16760-16-0 16760-18-2 16760-21-7 16760-22-8 16760-23-9
16802-49-6 16802-50-9 19060-65-2 19060-69-6 ***19060-73-2***
19060-74-3 19060-75-4 19060-76-5 19060-77-6
19060-78-7 19060-79-8 19060-80-1 19083-75-1 19083-76-2
19083-77-3 19083-78-4 19083-79-5 19083-80-8 19083-81-9
19083-82-0 19083-83-1 19083-84-2 19083-85-3 19083-86-4
19083-87-5 19083-88-6 19083-89-7 19083-90-0 19083-91-1
19083-92-2 19083-93-3 19083-96-6 19083-97-7 19083-98-8
19083-99-9 19084-00-5 19084-01-6 19084-02-7 19142-70-2
19142-71-3 19142-72-4
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(***neoplasm*** inhibition by)

IT ***19060-73-2 19060-74-3 19060-75-4***
19060-76-5
RL: ***BAC (Biological activity or effector, except adverse)***; BSU (Biological study, unclassified); ***THU (Therapeutic use)***; BIOL (Biological study); USES (Uses)
(***neoplasm*** inhibition by)

RN 19060-73-2 HCAPLUS

CN Terephthalanilide, 2-methoxy-4',4''-bis(3-pyridylcarbamoyl)- (8CI) (CA INDEX NAME)

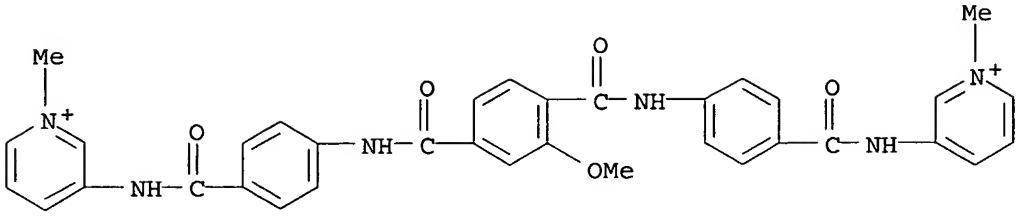


RN 19060-74-3 HCAPLUS

CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-methyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

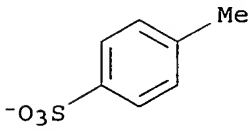
CM 1

CRN 47863-82-1
CMF C35 H32 N6 O5



CM 2

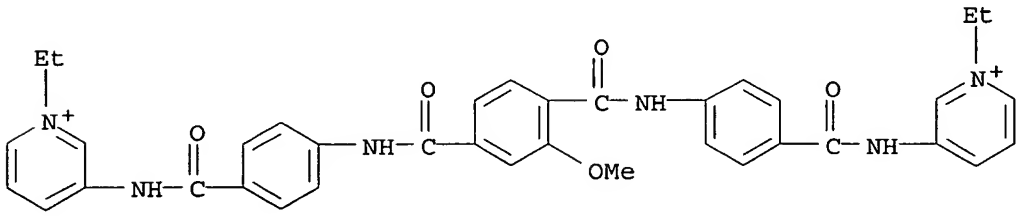
CRN 16722-51-3
CMF C7 H7 O3 S



RN 19060-75-4 HCAPLUS
CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-ethyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 47870-25-7
CMF C37 H36 N6 O5



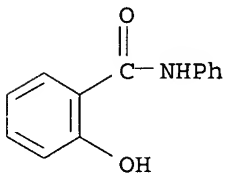
CM 2

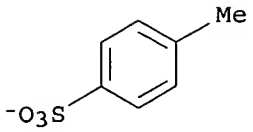
CRN 16722-51-3
CMF C7 H7 O3 S

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1126374		19620329	DE 1959-F29253	19590827 <--
GB 892263			GB	
US 3113067		19631203	US 1960-51286	19600823 <--

AB It is found that the title compds. are effective for combating water snails (gastropods). Other anti-snail compds. are known, but they have low solubility Their alkali salts are useful, except in brackish water, where they precipitate Compds. of this invention do not require solubility ***aids*** and do not precipitate in brackish water. A table shows comparative solys. A MeOH suspension of 25 g. 5,2'-dichloro-4'-nitrosalicylanilide (I) is treated with a MeOH solution of diethanolamine at 55° with stirring. The solution solidifies on cooling. This is washed and vacuum-dried to give 28 g. product, m. 186°. An aqueous suspension of 4.5 g. 5,2',5'-trichloro-4'-nitrosalicylanilide is treated with a water solution of 1,2-dimethylethanolamine. The salt ppts. and is washed and dried to give 5.2 g. product, m. 201°. I (50 g.) is mixed with monoethanolamine and warmed to give 57.3 g. salt, m. 204°. A mixture of DMSO and ethanolamine is combined with powdered I to give a H2O-soluble product. Similarly prepared are products from 5-bromo-2',5'-dichloro-4'-nitrosalicylanilide and HO(CH2)3NH2 (II), m. 209°, from 3-methyl-3',5,5'-trichloro-4'-nitrosalicylanilide and II, m. 189°, from 2',5,5'-trichloro-4'-nitroacetylsalicylanilide and MeNHCH2CH2OH, 149°, from 3',5,5'-trichloro-2'-nitrosalicylanilide and MeNHCH2CH2OH, m. 178°, and from 3-methyl-2',5,5'-trichloro-4'-nitroacetylsalicylanilide with MeCH(NH2)CH2CH2OH, m. 160 °.

INCL 120
CC 29 (Noncondensed Aromatic Compounds)
IT ***87-17-2***, Salicylanilide
(aci-nitro derivs., compds. with amino alcs.)
IT ***87-17-2***, Salicylanilide
(aci-nitro derivs., compds. with amino alcs.)
RN 87-17-2 HCAPLUS
CN Benzamide, 2-hydroxy-N-phenyl- (9CI) (CA INDEX NAME)

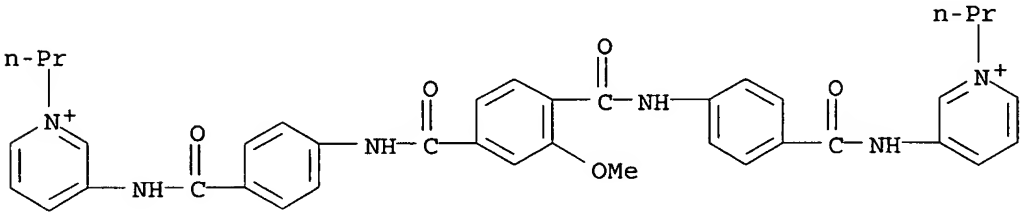




RN 19060-76-5 HCAPLUS
CN Pyridinium, 3,3'-[(2-methoxy-1,4-phenylene)bis(carbonylimino-4,1-phenylenecarbonylimino)]bis[1-propyl-, salt with 4-methylbenzenesulfonic acid (1:2) (9CI) (CA INDEX NAME)

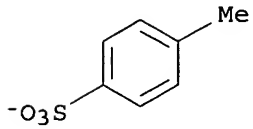
CM 1

CRN 47878-28-4
CMF C39 H40 N6 O5



CM 2

CRN 16722-51-3
CMF C7 H7 O3 S



L101 ANSWER 44 OF 44 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1962:449111 HCAPLUS <<LOGINID::20061006>>
DOCUMENT NUMBER: 57:49111
ORIGINAL REFERENCE NO.: 57:9751a-c,9752a
TITLE: Alkanolamine salts of salicylanilides
INVENTOR(S): Strufe, Reimer; Schraufstaetter, Ernst; Goennert, Rudolf
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: 3 pages
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION: